Enhancement of Antiferromagnetic Correlations below Superconducting Transition Temperature in Bilayer Superconductors

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(Dated: May 5, 2014)

Motivated by the recent experiment in multilayered cuprate superconductors reporting the enhancement of antiferromagnetic order below the superconducting transition temperature, we study the proximity effect of the antiferromagnetic correlation in a bilayer system and also examine the possibility of a coexistence of antiferromagnetic order and superconductivity. We present the result of mean field theory that is consistent with the experiment and supports the proximity effect picture.

PACS numbers: 74.78.Fk, 74.72.-h

I. INTRODUCTION

In the study of high-temperature superconductivity in the cuprates, there has been intense interest in the interplay between antiferromagnetism and superconductivity. The undoped parent compound, which is a Mott insulator, is an antiferromagnetic (AF) long-range ordered state. Upon carrier doping, the AF state is converted into the high-temperature superconducting (SC) state. In the mechanism of superconductivity, the AF correlation is believed to play an important role. In order to investigate the AF correlation effect on superconductivity, the cuprates, there has been intense interest in the interplay between antiferromagnetism and superconductivity. We present the result of mean field theory that is consistent with the experiment and supports the proximity effect picture.

From nuclear magnetic resonance (NMR) experiments it was suggested that SC moments survived even in a SC phase. A possibility of a phase separation is ruled out because the NMR signal associated with the par-...
Here $c_{i,k\sigma}^\dagger (c_{i,k\sigma})$ creates (annihilates) electrons with in-plane momentum $k$ and spin $\sigma$ at layer $l$. We assume that the interlayer hopping matrix $t_p$ is independent of $k$. The Hamiltonian for the $l$ layer is

$$H_l = \sum_{k,\sigma} \xi_k c_{i,k\sigma}^\dagger c_{i,k\sigma} - V_l \sum_j \left(c_{i,j\sigma}^\dagger c_{i,j\sigma} - c_{i,j\sigma}^\dagger c_{i,j\sigma}\right)^2 - g_l \sum_{k \neq k'} f(k) f(k') c_{i,k\sigma}^\dagger c_{i,-k\sigma} c_{i,-k'\sigma} c_{i,k'\sigma},$$

with $\xi_k = -2t(\cos k_x + \cos k_y) - \mu$. (Hereafter we set the lattice constant to unity.) The hopping of electrons within each layer is restricted to the nearest neighbors given by $t$. Energies are measured in units of $t$ in the following analysis. We focus on the half-filling case in each layer so that we set the chemical potential $\mu = 0$. This means that we neglect charge redistribution between the two layers. The second term of $H_l$ describes the AF interaction. The operator $c_{i,j\sigma}^\dagger c_{i,j\sigma}$ creates (annihilates) electrons at site $j$. The third term of $H_l$ with $f(k) = (\cos k_x - \cos k_y)/2$ describes the interaction for $d_{x^2-y^2}$-wave pairing.

We define the $d$-wave SC order parameter in the $l$ layer with $N$ sites by

$$\Delta_l = \frac{1}{N} \sum_k \Delta_l(k),$$

with

$$\Delta_l(k) = f(k) c_{i,k\uparrow} c_{i,-k\downarrow}.$$

The AF order parameter in the $l$ layer is defined by

$$m_l = \frac{1}{2N} \sum_{k \in \text{RBZ}} (c_{i,k\sigma}^\dagger c_{i,+Q\sigma} - c_{i,k\sigma}^\dagger c_{i,k+Q\sigma}) + \text{c.c.},$$

where the summation with respect to $k$ is taken over the reduced Brillouin zone $|k_x| + |k_y| < \pi$ and the nesting vector is $Q = (\pi, \pi)$. By using the order parameters, the mean field Hamiltonian at the $l$ layer reads

$$H_{l}^{mf} = \sum_{k \in \text{RBZ}} C_{lk} M_{lk} C_{lk} + 4NV m_l^2 + N g_l |\Delta_l|^2,$$

where

$$C_{lk} = \begin{pmatrix} c_{l,k\uparrow} & c_{l,k+Q\uparrow} & c_{l,-k\downarrow} & c_{l,-k-Q\downarrow} \end{pmatrix}^T$$

and

$$M_{lk} = \begin{pmatrix} \xi_k & -4m_l V_l & -g_l \Delta_l(k) & 0 \\ -4m_l V_l & \xi_{k+Q} & 0 & -g_l \Delta_l(k) \\ -g_l \Delta_l(k)^* & 0 & -\xi_k & -4m_l V_l \\ 0 & -g_l \Delta_l(k)^* & -4m_l V_l & -\xi_{k+Q} \end{pmatrix}. $$

$$\Delta_l(k)$$

Based on the mean field Hamiltonian of the whole system, $\sum_l H_{l}^{mf} + H_{\perp}$, we solve the mean-field Eqs. (4) and (6) numerically using the $100 \times 100$ discretized Brillouin zone.

### III. COEXISTENCE PHASE IN SINGLE LAYER SYSTEM

Before going into the analysis of the bilayer system, we examine a coexisting phase in a single layer system described by $H_l^{mf}$. Reflecting the difference in symmetry between the AF gap created by $m_l \neq 0$ and the SC gap $\Delta_l$, the coexistence phase of SC and AF orders can be stabilized.\cite{14,15} The situation is similar to the slave-boson mean field theory of the $t-J$ model\cite{16} and the Hubbard model in the strong-coupling limit.\cite{17}

Figure 1(a) shows the parameter range of $g \equiv g_1$ for the coexistence phase at $V \equiv V_1 = 0.5$. For $g < 5.0$ the system is a pure AF state while for $g > 6.3$ the system is a pure SC state.\cite{2} So the coexistence phase appears for $5.0 < g < 6.3$. For the case of $V = 0.4$, the parameter for the coexistence changes as $3.7 < g < 4.5$. In order to confirm that the state with $\Delta \neq 0$ and $m \neq 0$ is the global minimum of the free energy, we computed the following energy at $T = 0$ for $0 \leq \Delta \leq 0.2$ and $0 \leq m \leq 0.25$:

$$E = \sum_{\alpha,E_{\alpha}<0} E_{\alpha} + 4N V m^2 + N g |\Delta|^2,$$

where $\alpha$ runs over all the eigenstates of the mean field Hamiltonian and $E_{\alpha}$ are the eigenenergies. We examined several cases and confirmed that the coexistence phase solution corresponds to the global minimum of the energy. We examined the $s$-wave case as well, but there is no coexistence phase.

There are two types of coexistence phases. One is the phase with strong AF order and weak SC order, resulting in the AF transition temperature $T_{AF} > T_c$, and the other is the phase with $T_{AF} < T_c$. Figure 1(b) shows the temperature dependence of the order parameters in the coexistence phase with $T_{AF} > T_c$ at $g = 5$ and $V = 0.5$. For comparison, the pure AF case at $g = 0$ and $V = 0.5$ and the pure SC case at $g = 5$ and $V = 0$ are also shown. For this choice of the parameters, $T_{AF}$ is slightly higher than $T_c$. Therefore, the system first exhibits AF order upon decreasing temperature. $T_c$ is somewhat reduced because of the presence of AF order. The occurrence of the SC order also affects the AF order: the temperature dependence of $m$ in Fig. 1(b) deviates from the pure AF case at $T_c$, resulting in the reduction of $m$. This behavior is in contrast to the case of the multilayer cuprates where the enhancement of the AF order is observed.\cite{23} We note that, in the coexistence phase with $T_c > T_{AF}$, $T_c$ is the same as the value of the pure SC case but $T_{AF}$ is reduced from the pure AF case value.

### IV. PROXIMITY EFFECT IN BILAYER SYSTEM

In this section, we study the bilayer system. Our purpose is twofold. First, we study the proximity effect in the bilayer system. Second, we examine the stability of
the coexistence phase in a single layer under the presence of inter-layer tunneling.

To start with, we examine the interlayer tunneling effect. Depending on the value of \( t_p \), there are a strong \( t_p \) regime and a weak \( t_p \) regime. Figure 2 shows the \( t_p \) dependence of the AF order parameter \( m_1 \) and \( m_2 \) at \( V_1 = 0.4 \) and \( V_2 = 0.5 \) with \( g_1 = g_2 = 0 \). For \( t_p < 0.22 \), we see that the values of the order parameters are not so much affected by the increase of \( t_p \). This weak \( t_p \) regime is not suitable for describing multilayer systems because each layer is almost independent. In fact, the change of \( m_1 \) and \( m_2 \) in the weak \( t_p \) regime is described by the second-order perturbation theory with respect to \( t_p \). At \( t_p = 0.22 \), there is a first order transition between the weak \( t_p \) regime and the strong \( t_p \) regime as shown in Fig. 3. For \( t_p > 0.22 \), the order parameters exhibit strong \( t_p \) dependence. In this strong \( t_p \) regime, \( t_p \) is larger than the excitation gap created by AF order. Therefore, the order parameters are reduced due to the change of the Fermi-surface topology. In the large \( t_p \) limit, the noninteracting single-body electron states are well described by the bonding state and the anti-bonding state. The Fermi surface splits into two pockets centered at the \( \Gamma \) point and \( M \) point. Qualitatively similar behaviors are found in the \( t_p \) dependence of the SC order parameters. In the following analysis, we focus on this strong \( t_p \) regime and set \( t_p = 0.3 \).

Now we investigate the bilayer system. We consider three cases. In all cases, we assume \( V_2 = 0.5 \) and \( g_2 = 0 \) for \( l = 2 \). Therefore, the intrinsic order in the \( l = 2 \) layer is restricted to AF order. For the \( l = 1 \) layer, we assume \( g_1 \geq 3 \) and \( V_1 \geq 0 \).

The three cases are (i) \( V_1 = 0 \), (ii) \( V_1 = 0.4 (< V_2) \), and (iii) \( V_1 = 0.6 (> V_2) \). It turns out that the ground state of case (i) consists of SC order in the \( l = 1 \) layer and AF order in the \( l = 2 \) layer when \( g_1 \geq 3.7 \). The ground states of cases (ii) and (iii) are the coexistence state of SC and AF orders in the \( l = 1 \) layer and only AF order in the \( l = 2 \) layer. Cases (ii) and (iii) are distinguished by the strength of the AF order in the two layers: \( m_1 < m_2 \) in case (ii), while \( m_1 > m_2 \) in case (iii).

Figure 3(a) is a schematic view of case (i). The temperature dependence of the order parameters is shown in Figs. 3(b)-3(d) for different values of \( g_1 \). For \( g_1 = 3 \), there is no SC order in the \( l = 1 \) layer. Intrinsic AF order \( m_2 \) appears in the \( l = 2 \) layer for \( T < T_{AF} = 0.14 \) as shown in Fig. 3(d). As a result of the proximity effect, a finite value of \( m_1 \) is induced as shown in Fig. 3(c). This induced \( m_1 \) decreases with increasing \( g_1 \) because the intrinsic SC order by \( g_1 \) competes with the induced AF order. On the other hand, the intrinsic AF order \( m_2 \) in the \( l = 2 \) layer increases with increasing \( g_1 \). At \( g_1 = 4.0 \) there is a SC transition in the \( l = 1 \) layer as shown in Fig. 3(b). In the presence of the non-zero SC order parameter, \( \Delta_1 \), in the \( l = 1 \) layer, a finite value of \( \Delta_2 \) is induced in the \( l = 2 \) layer (not shown) because of the proximity effect. The SC transition affects \( m_2 \). As shown in Fig. 3(d), there is a clear enhancement of \( m_2 \) below the SC transition temperature \( T_c = 0.06 \) for the case of \( g_1 = 4 \). A similar enhancement is also found in the case of \( g_1 = 5 \) below \( T_c = 0.12 \). This enhancement of \( m_2 \) below \( T_c \) is consistent with the experiment in the multilayer cuprate. For
The enhancement of AF order below $T_c$ is also found in the case (ii) (Fig. 4(a)). Figures 4(b)-(d) show the temperature dependence of the order parameters for different values of $g_1$. For the case of $g_1 < 5.1$, there is no intrinsic SC order in the $l = 1$ layer. For the case of $g_1 = 5.2$, there is a SC transition at $T_c = 0.13$. Below $T_c$, $m_2$ is clearly enhanced, although the enhancement is much reduced compared to the case (i). Similar behaviors are observed for $g_1 \geq 5.1$. Again this behavior is consistent with the experiment.\textsuperscript{12}

Now we examine the case (iii) (Fig. 5(a)). The temperature dependence of the order parameters is shown in Figs. 5(b)-(d). In this case, we observe quite different behaviors of the order parameters compared to the cases (i) and (ii). In particular, the superconducting transition temperature $T_c$ is always larger than the AF transition temperature $T_{AF}$. There is no coexistence phase when $T_c < T_{AF}$. For $T_{AF} < T < T_c$, $\Delta_1$ increases as $T$ decreases as shown in Fig. 5(b). Below $T_{AF}$, $\Delta_1$ is suppressed. Furthermore, the coexistence phase is limited to a finite range of temperature for $6.7 \leq g_1 \leq 7.1$.\textsuperscript{12}
Meanwhile the order parameters $m_1$ and $m_2$ increase monotonically as the temperature decreases as shown in Figs. 5(c) and (d). These temperature dependences are qualitatively different from the experimentally observed one. From this observation one may conclude that it is unlikely that there is a coexistence phase of intrinsic SC and AF orders in a layer among coupled multilayers. Although the coexistence phase of AF and SC orders appears in all cases (i)-(iii), the origin of AF order in the SC layer is different. What makes the difference between the case (iii) and the case (ii) is that in the case (iii) AF order in the $l=1$ layer with SC is intrinsic order but not induced by the other layer. Meanwhile in the case (ii) AF order in the $l=1$ layer with SC is induced order by AF order in the $l=2$ layer due to the proximity effect.

So far we have studied the system with the electron hopping restricted to the nearest neighbors. In order to examine the system with a realistic Fermi surface we consider the model with

$$
\xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu. \tag{10}
$$

Here we choose $t'/t = -0.20$ and $t''/t = 0.10$. We take the chemical potential as $\mu = -0.839$, which corresponds to 10% doping in the normal and non-magnetic state. The result for the case (i) above with $V_1 = 0$ and $V_2 = 0.8$ is shown in Fig. 6. The temperature dependence of the order parameters is shown in Figs. 6(b)-(d) for different values of $g_1$. We observe qualitatively similar behaviors of the order parameters to the case (i) shown in Fig. 4. There is a clear enhancement of $m_2$ below the SC transition. Intrinsic AF order $m_2$ appears in the $l=2$ layer for $T < T_{AF} = 0.23$ as shown in Fig. 6(d). This intrinsic order is enhanced below the SC transition. For example, there is the SC transition at $T = 0.15$ for $g_1 = 5.0$ as shown in Fig. 6(b). For $T < 0.15$, $m_2$ is enhanced compared with the $g_1 = 0$ case. Meanwhile, $m_1$ is suppressed as shown in Fig. 6(c). The exceptional case is $g_1 = 4.0$. The temperature dependence of $m_2$ is similar to the other cases but the temperature dependence of $m_1$ is qualitatively different. The value of $m_1$ is enhanced below the SC transition. This discrepancy is probably associated with the change of the Fermi surface shape.

V. SUMMARY

To summarize, we have studied the proximity effect and the possibility of coexistence of AF and SC orders in a bilayer system. Our mean field theory suggests that the experimentally observed enhancement of AF order below $T_{c12}$ is associated with the proximity effect. In contrast, if we assume a coexistence phase in a layer among coupled multilayers, the temperature dependence of the order parameters is qualitatively different from the experimentally observed one.

We believe that this result is not so much affected by the shape of the Fermi surface. As we have shown in Fig. 3 the result for a realistic Fermi surface with finite doping is qualitatively the same as that for the half-filling case. So we expect qualitatively the same proximity effect as long as we neglect the possibility of stabilizing other orders, such as a charge-density wave or the so-called $\pi$-triplet pairing. The absence of the $\pi$-triplet pairing is the unique property of the half-filling case with $t' = t'' = 0$. However, there is no experimental evidence for the $\pi$-triplet pairing to the best of our knowledge.
FIG. 6. (Color online) (a) Schematic view of the system for the case (i) with $V_1 = 0$ and $V_2 = 0.8$. The temperature dependence of the SC order parameter $\Delta_1$ in layer-1 (b), the AF order parameter $m_1$ in layer-1 (c), and the AF order parameter $m_2$ in layer-2 (d) for various $g_1$.

ACKNOWLEDGMENT

This work was supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science, and Technology of Japan; the Global Center Of Excellence (COE) Program “The Next Generation of Physics, Spun from University and Emergence”; and the Yukawa Institutional Program for Quark-Hadron Science at Yukawa Institute of Theoretical Physics.

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In Fig. 1(a) $m$ has tiny values for $g > 6.3$ but this is a finite size effect. By increasing the number of Brillouin zone points taken in the numerical calculation, the finite values of $m$ for $g > 6.3$ are suppressed.

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