Enhancement of antiferromagnetic correlations below the superconducting transition temperature in bilayer superconductors

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(Received 1 March 2012; published 18 May 2012)

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.

DOI: 10.1103/PhysRevB.85.184523 PACS number(s): 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, multilayer systems are useful. In multilayer systems, the number of CuO_2 layers per unit cell, n, takes $n \geqslant 2$. From systematic studies of the n dependence of SC transition temperature T_c, it is found that the maximum T_c is obtained[1,2] for the case of $n = 3,4$. Since coupling between the CuO_2 planes within the unit cell is stronger than that between the CuO_2 planes in different unit cells, the AF correlation can be strong in multilayer systems. There is also charge imbalance over the CuO_2 layers as revealed by the ^{63}Cu Knight shifts, and thus the multilayer systems form a natural heterostructure at an intermediate carrier-concentration region.[3]

From nuclear magnetic-resonance (NMR) experiments it was suggested that AF moments survived even in a SC phase.[4–7] A possibility of a phase separation is ruled out because the NMR signal associated with the paramagnetic state was not observed.[5] An important issue here is whether SC order coexists with AF order[8,10,11] or not. Recently, Shimizu *et al.* studied the temperature dependence of the AF moment in a five-layered cuprate $Ba_2Ca_4Cu_5O_{10}(F,O)_2$ by NMR measurements.[12] They reported that the AF moment in the outer layer is enhanced below T_c. Such an enhancement of the AF moment below T_c does not appear in the coexistence phase of other superconductors such as iron arsenide superconductor $Ba_2(Fe_{1-x}Co_x)_2As_2$, where the AF moment reduces at T_c.[13] Therefore, the enhancement seen in the five-layered cuprate is not necessarily common to all of the coexistence phase of superconductors. Noting that the iron arsenide is a single layer system, we may speculate that the multilayer nature is essential for the enhancement and thus need to clarify the mechanism of the AF moment enhancement triggered by the SC transition under the presence of multilayers.

In this paper, we study the interplay between SC and AF orders within a mean-field theory. To describe a multilayer system, where there are two types of layers associated with outer planes and inner planes, we consider a bilayer system with different electronic correlations in each layer. By controlling interaction parameters for the AF correlation and the SC correlation, we study the proximity effect between two layers with different order and also examine the possibility of coexistence of SC and AF orders. We find that the proximity effect leads to an enhancement of AF order below the SC transition temperature that is consistent with the experiment.[12] By contrast, we find qualitatively different behaviors of the order parameters for the coexistence case.

This paper is organized as follows. In Sec. II, we introduce the bilayer Hamiltonian and describe the mean-field theory. In our model, a coexistence phase of SC and AF orders is possible within a single layer. This coexistence phase is described in Sec. III. In Sec. IV, we describe the results about the proximity effect in the bilayer system. We show that the temperature dependence of the AF moment is consistent with the experiment.[12] We also examine coexistence phases and show that the temperature dependence of the order parameters is quite different from the experiment. Finally, Sec. V is devoted to summary and discussions.

II. MODEL AND FORMALISM

We consider a bilayer system with interactions which stabilize SC and/or AF order. The two layers are coupled through an interlayer tunneling. The Hamiltonian is given by

$$\mathcal{H} = \sum_{l=1,2} \mathcal{H}_l + \mathcal{H}_\perp, \tag{1}$$

where the interlayer tunneling term $\mathcal{H}_\perp$ is

$$\mathcal{H}_\perp = -t_p \sum_{\boldsymbol{k},\sigma} \left(c^\dagger_{1,\boldsymbol{k}\sigma} c_{2,\boldsymbol{k}\sigma} + \text{H.c.} \right). \tag{2}$$

Here $c^\dagger_{l,\boldsymbol{k}\sigma}$ ($c_{l,\boldsymbol{k}\sigma}$) creates (annihilates) electrons with in-plane momentum $\boldsymbol{k}$ and spin σ at layer l. We assume that the interlayer hopping matrix t_p is independent of $\boldsymbol{k}$. The Hamiltonian for the l layer is

$$\mathcal{H}_l = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^\dagger_{l,\boldsymbol{k}\sigma} c_{l,\boldsymbol{k}\sigma} - V_l \sum_j \left(c^\dagger_{lj\uparrow} c_{lj\uparrow} - c^\dagger_{lj\downarrow} c_{lj\downarrow} \right)^2 - g_l \sum_{\boldsymbol{k}\neq\boldsymbol{k}'} f(\boldsymbol{k}) f(\boldsymbol{k}') c^\dagger_{l,\boldsymbol{k}\uparrow} c^\dagger_{l,-\boldsymbol{k}\downarrow} c_{l,-\boldsymbol{k}'\downarrow} c_{l,\boldsymbol{k}'\uparrow}, \tag{3}$$

with $\xi_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y) - \mu$. (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-filing 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 $\mathcal{H}_l$ describes the AF interaction. The operator $c^\dagger_{lj\sigma}$ $(c_{lj\sigma})$ creates (annihilates) electrons at site j. The third term of $\mathcal{H}_l$ with $f(\boldsymbol{k}) = (\cos k_x - \cos k_y)/2$ 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

$$\Delta_l = \frac{1}{N}\sum_{\boldsymbol{k}} \Delta_l(\boldsymbol{k}), \tag{4}$$

with

$$\Delta_l(\boldsymbol{k}) = f(\boldsymbol{k})\langle c_{l,\boldsymbol{k}\uparrow} c_{l,-\boldsymbol{k}\downarrow}\rangle. \tag{5}$$

The AF order parameter in the l layer is defined by

$$m_l = \frac{1}{2N}\sum_{\boldsymbol{k}\in \mathrm{RBZ}} \langle c^\dagger_{l,\boldsymbol{k}\uparrow} c_{l,\boldsymbol{k}+\boldsymbol{Q}\uparrow} - c^\dagger_{l,\boldsymbol{k}\downarrow} c_{l,\boldsymbol{k}+\boldsymbol{Q}\downarrow}\rangle + \text{c.c.}, \tag{6}$$

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

$$\mathcal{H}^{\mathrm{mf}}_l = \sum_{\boldsymbol{k}\in \mathrm{RBZ}} C^\dagger_{l\boldsymbol{k}} M_{l\boldsymbol{k}} C_{l\boldsymbol{k}} + 4NV_l m_l^2 + Ng_l|\Delta_l|^2, \tag{7}$$

where $C_{l\boldsymbol{k}} = (c_{l,\boldsymbol{k}\uparrow}\ c_{l,\boldsymbol{k}+\boldsymbol{Q}\uparrow}\ c^\dagger_{l,-\boldsymbol{k}\downarrow}\ c^\dagger_{l,-\boldsymbol{k}-\boldsymbol{Q}\downarrow})^T$ and

$$M_{l\boldsymbol{k}} = \begin{pmatrix} \xi_{\boldsymbol{k}} & -4m_lV_l & -g_\ell\Delta_l(\boldsymbol{k}) & 0 \\ -4m_lV_l & \xi_{\boldsymbol{k}+\boldsymbol{Q}} & 0 & -g_\ell\Delta_l(\boldsymbol{k}) \\ -g_\ell\Delta_l(\boldsymbol{k})^* & 0 & -\xi_{\boldsymbol{k}} & -4m_lV_l \\ 0 & -g_\ell\Delta_l(\boldsymbol{k})^* & -4m_lV_l & -\xi_{\boldsymbol{k}+\boldsymbol{Q}} \end{pmatrix}. \tag{8}$$

Based on the mean-field Hamiltonian of the whole system, $\sum_l \mathcal{H}^{\mathrm{mf}}_l + \mathcal{H}_\perp$, we solve the mean-field Eqs. (4) and (6) numerically using the 100×100 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 $\mathcal{H}^{\mathrm{mf}}_l$. Reflecting the difference in symmetry between the AF gap created by $m_l \neq 0$ and the SC gap Δ_l, the coexistence phase of SC and AF orders can be stabilized.[14,15] The situation is similar to the slave-boson mean-field theory of the t-J model[16] and the Hubbard model in the strong-coupling limit.[8]

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.[9] 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 $0 \leqslant \Delta \leqslant 0.2$ and $0 \leqslant m \leqslant 0.25$:

$$E = \sum_{\alpha, E_\alpha < 0} E_\alpha + 4NVm^2 + Ng|\Delta|^2, \tag{9}$$

where α runs over the all eigenstates of the mean-field Hamiltonian and E_α 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.

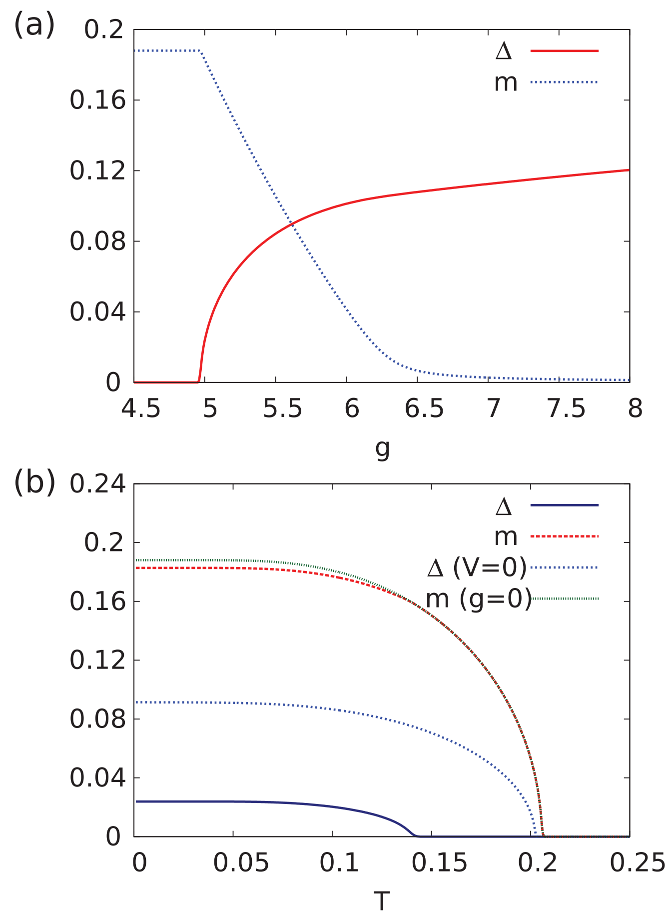

FIG. 1. (Color online) (a) The AF order parameter m and the d-wave SC order parameter Δ vs the SC interaction parameter g at $V = 0.5$ in the single layer system at $T = 0$. (b) The temperature dependence of the order parameters in the coexistence phase for $g = 5$ and $V = 0.5$. For comparison we show the pure SC case ($g = 5$ and $V = 0$) and the pure AF case ($g = 0$ and $V = 0.5$) as well.

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 $T_{\mathrm{AF}} > T_{\mathrm{c}}$, and the other is the phase with $T_{\mathrm{AF}} < T_{\mathrm{c}}$. Figure 1(b) shows the temperature dependence of the order parameters in the coexistence phase with $T_{\mathrm{AF}} > T_{\mathrm{c}}$ 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

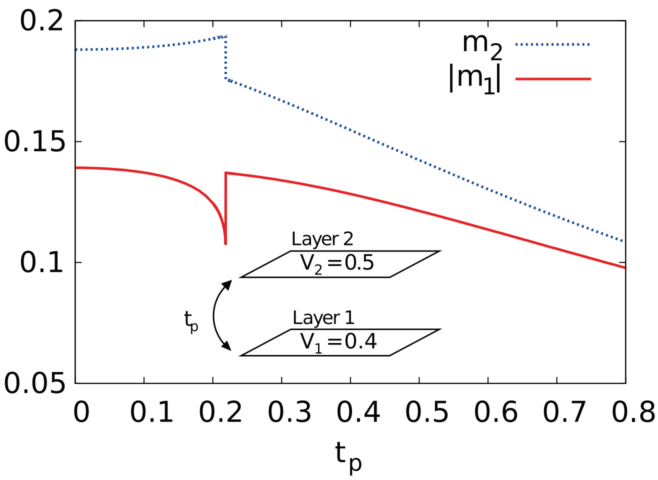

FIG. 2. (Color online) The AF order parameters m_1 and m_2 vs the interlayer hopping parameter t_p in the bilayer system for $V_1 = 0.4$ and $V_2 = 0.5$. Inset: a schematic view of the system.

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.[12] 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 interlayer 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 parameters 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. 2. 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 antibonding state. The Fermi surface splits into two pockets centered at the Γ 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 $g_1 \geqslant 3$ and $V_1 \geqslant 0$.

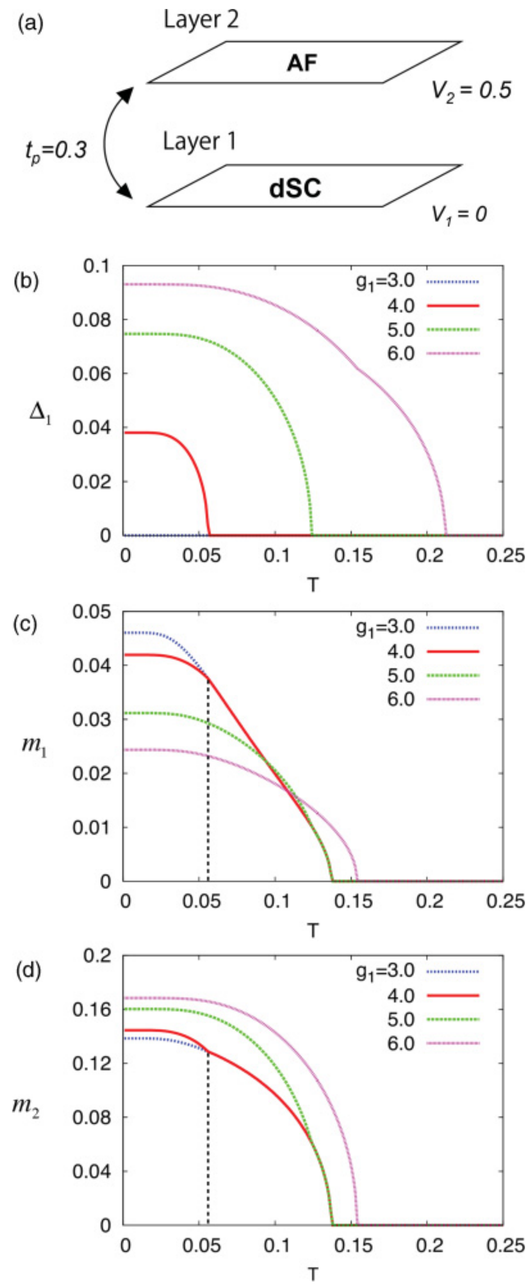

FIG. 3. (Color online) (a) Schematic view of the system for case (i) (see the text) and the temperature dependence for various g_1 of (b) the SC order parameter Δ_1 in layer 1, (c) the AF order parameter m_1 in layer 1, and (d) the AF order parameter m_2 in layer 2. The vertical dashed line represents T_c in the case of $g_1 = 4.0$.

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 $g_1 \geqslant 3.7$. 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 nonzero SC order parameter, Δ_1, in the $l = 1$ layer, a finite value of Δ_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.[12] For $g_1 = 6$ this enhancement is masked because T_c is higher than T_{AF}.

The enhancement of AF order below T_c is also found in case (ii) [Fig. 4(a)]. Figures 4(b)–4(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 case (i). Similar behaviors are observed for $g_1 \geqslant 5.1$. Again this behavior is consistent with the experiment.[12]

Now we examine case (iii) [Fig. 5(a)]. The temperature dependence of the order parameters is shown in Figs. 5(b)–5(d). In this case, we observe quite different behaviors of the order parameters compared to 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 $T_{AF} < T < T_c$, Δ_1 increases as T decreases as shown in Fig. 5(b). Below T_{AF}, Δ_1 is suppressed. Furthermore, the coexistence phase is limited to a finite range of temperature for $6.7 \leqslant g_1 \leqslant 7.1$. Meanwhile the order parameters m_1 and m_2 increase monotonically as the temperature decreases as shown in Figs. 5(c) and 5(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 case (iii) and case (ii) is that in case (iii) AF order in the $l = 1$ layer with SC is intrinsic order but not induced by the other layer. Meanwhile in 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,[17–19] we consider the model with

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

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 nonmagnetic state. The result for 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)–6(d) for different values of g_1. We observe qualitatively similar behaviors of the order parameters to case (i) shown in Fig. 3. 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).

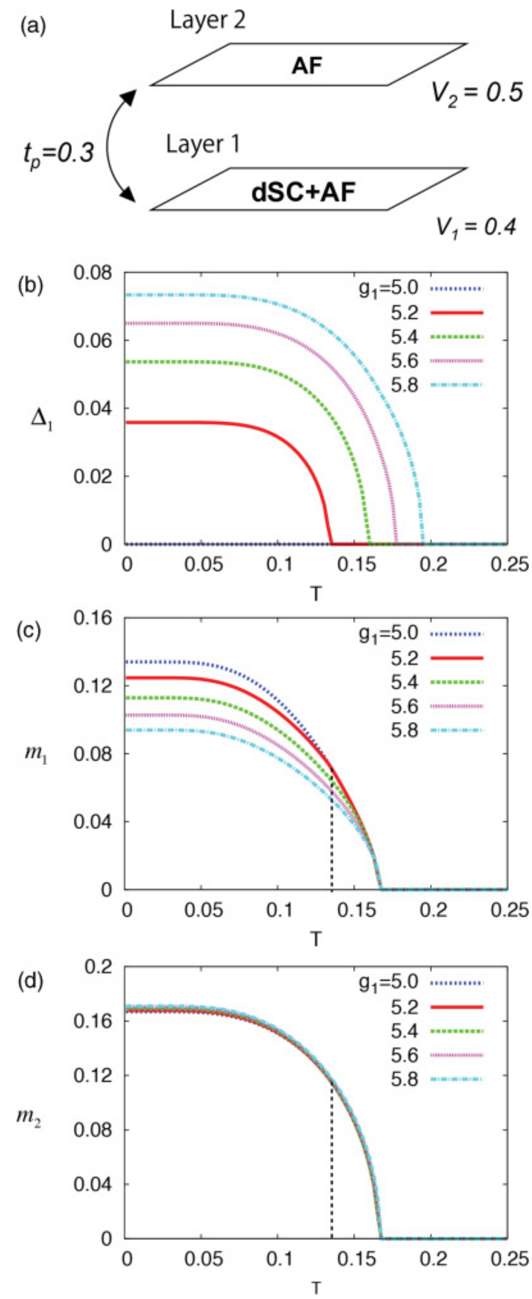

FIG. 4. (Color online) (a) Schematic view of the system for case (ii) (see the text) and the temperature dependence for various g_1 of (b) the SC order parameter Δ_1 in layer 1, (c) the AF order parameter m_1 in layer 1, and (d) the AF order parameter m_2 in layer 2. The vertical dashed line represents T_c in the case of $g_1 = 5.2$. The inset in (d) is the enlarged drawing of m_2 at low temperatures for $g_1 = 5.0$,5.2.

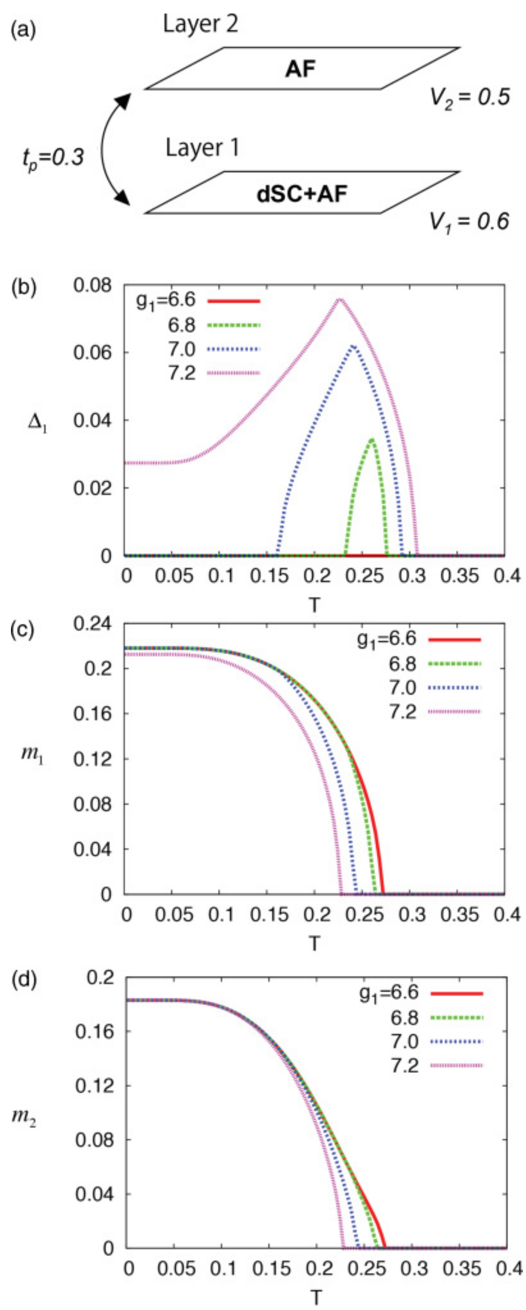

FIG. 5. (Color online) (a) Schematic view of the system for case (iii) (see the text) and the temperature dependence for various g_1 of (b) the SC order parameter Δ_1 in layer 1, (c) the AF order parameter m_1 in layer 1, and (d) the AF order parameter m_2 in layer 2.

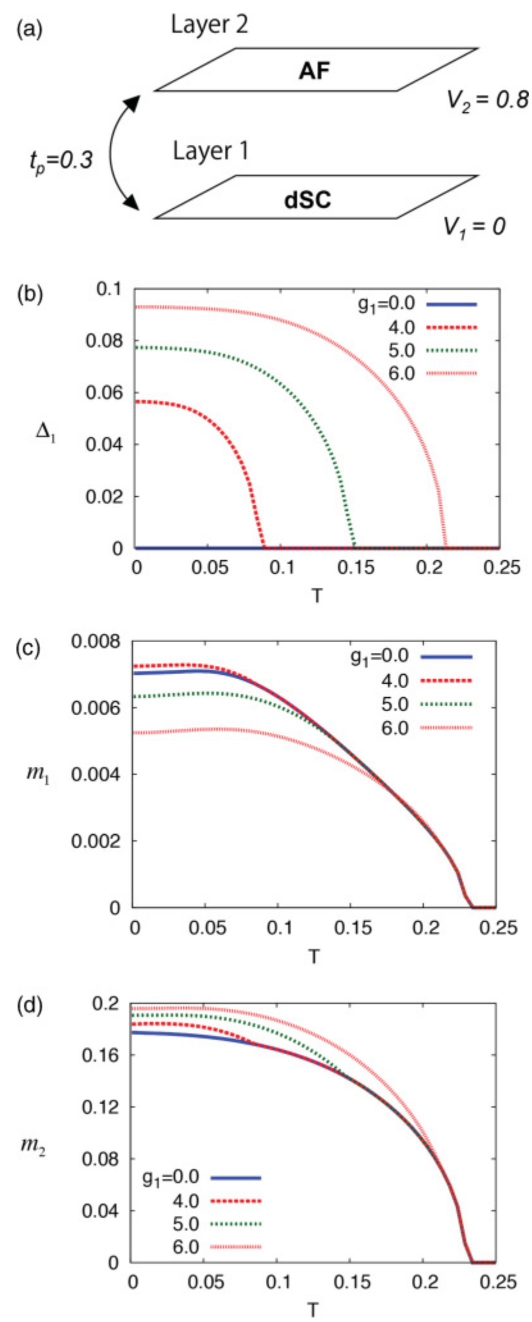

FIG. 6. (Color online) (a) Schematic view of the system for case (i) with $V_1 = 0$ and $V_2 = 0.8$ and the temperature dependence for various g_1 of (b) the SC order parameter Δ_1 in layer 1, (c) the AF order parameter m_1 in layer 1, and (d) the AF order parameter m_2 in layer 2.

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_c[12] 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. 6, 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 π-triplet pairing.[14,20,21] The absence of the π-triplet pairing is the unique property of the half-filling case with $t' = t'' = 0$. However, there is no experimental evidence for the π-triplet pairing to the best of our knowledge.

ACKNOWLEDGMENTS

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 (YITP).

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[9] 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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