Gossamer superconductivity and antiferromagnetism in the *t-J-U* model

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The *d*-wave superconductivity (dSC) and antiferromagnetism are analytically studied in a renormalized mean-field theory for a two-dimensional *t-J* model plus an on-site repulsive Hubbard interaction *U*. The purpose of introducing the *U* term is to partially impose the no-double-occupancy constraint by employing the Gutzwiller approximation. The phase diagrams as functions of doping δ and *U* are studied. Using the standard value of $t/J=3.0$ and in the large-*U* limit, we show that the antiferromagnetic (AF) order emerges and coexists with the dSC in the underdoped region below the doping $\delta\sim 0.1$. The dSC order parameter increases from zero as the doping increases and reaches a maximum near the optimal doping $\delta\sim 0.15$. In the small-*U* limit, only the dSC order survives while the AF order disappears. As *U* increases up to a critical value, the AF order shows up and coexists with the dSC in the underdoped regime. At half-filling, the system is in the dSC state for small *U* and becomes an AF insulator for large *U*. Within the present mean-field approach, we show that the ground-state energy of the coexistent state is always lower than that of the pure dSC state.

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I. INTRODUCTION

In spite of tremendous theoretical and experimental efforts dedicated to the studies of the anomalous properties of high-T_c superconductors (HTS), a full understanding of these materials is still far from the final stage. As a basic point, it is known that much of the physics should come from the competition between the *d*-wave superconductivity (dSC) and antiferromagnetism. Experimentally, it is generally suggested that the ground state evolves from the antiferromagnetic (AF) state to that of the dSC order as the carrier density increases.[1] However, since the early days of HTS, there also have been persistent reports of the coexistence of the dSC and AF orders[2–8] in various cuprate samples. Especially in the recent neutron-scattering experiments, the commensurate AF order has been observed in the underdoped superconducting $YBa_2Cu_3O_{6.5}$, providing unambiguous evidence for an unusual spin-density-wave state coexisting with superconductivity (dSC).[6] Therefore, it is necessary to develop a microscopic theory in which both the antiferromagnetism and the dSC are treated equally in order to understand the ground-state property of the cuprate superconductors.

Theoretically, it has been widely accepted that the essential physics of cuprates can be effectively described by the two-dimensional Hubbard model or its equivalent *t-J* model in the large-*U* limit.[9,10] Using the variational Monte Carlo (VMC) method, several groups proposed wave functions with coexisting AF and dSC orders and found that the coexisting state has a lower energy than either the pure dSC order or the pure AF state in the underdoped regime.[11–14] Although the slave particle mean-field theory for the *t-J* model was originally introduced to investigate the formation of the RVB state or the superconducting order,[9,15–18] it also has been applied to study the coexistence of the dSC and AF orders in this system.[19,20] Stimulated by the idea of the "gossamer superconductors" proposed by Laughlin,[21] Zhang and co-workers[22] employed the *t-J-U* model with the Gutzwiller projected wave function[23] to investigate the superconducting order parameter and the electron pairing gap (or the RVB order parameter). There[22] the on-site Coulomb interaction *U* is introduced to partially impose the no-double-occupancy constraint for the strongly correlated electron systems. In the large-*U* limit, their result[22] is consistent with that of Kotliar and Liu[16] using the slave boson mean-field approach for the *t-J* model.

Following Ref. 22, we report a further investigation of the same model by taking the AF order explicitly into consideration. Within the Gutzwiller renormalized mean-field theory, we find that for large Coulomb repulsion *U*, there is a coexistence between AF and dSC orders below the doping level $\delta\sim 0.1$. The coexisting state always has a lower energy than that of the pure dSC state. The dSC order parameter increases from zero as the doping increases in the underdoped region and then reaches a maximum near the optimal doping $\delta\sim 0.15$, after which it decreases to zero at $\delta\sim 0.35$ with increasing doping. When the magnitude of *U* is reduced, the AF order parameter decreases very quickly with increasing doping, and the coexistent region is squeezed toward the low doping regime until it disappears for $U<5.3t$, where the "gossamer superconductivity" is found even at half-filling.

The paper is organized as follows. In Sec. II, we outline the theoretical framework. The *t-J-U* model is introduced and the Gutzwiller variational approach is formulated. A renormalized Hamiltonian is obtained and further studied within the mean-field theory. In Sec. III, our numerical results are displayed and compared with those from other theories and experiments. In Sec. IV, a summary of the paper will be given.

II. THEORETICAL FRAMEWORK

We start from the *t-J-U* model on a square lattice,[22]

$$H = H_t + H_s + H_U, \tag{1}$$

with

$$H_t = -t\sum_{i\hat{\eta}\sigma} (C^{\dagger}_{i\sigma}C_{i+\hat{\eta}\sigma} + \mathrm{H.c.}),$$

$$H_s = J\sum_{i\hat{\eta}} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{\eta}},$$

$$H_U = U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{2}$$

where $\hat{\eta}=\hat{x}$ and $\hat{y}$, $C^{\dagger}_{i\sigma}(C_{i\sigma})$ is the electron creation (annihilation) operator, $\mathbf{S}_i=\Sigma_{\sigma\sigma'}C^{\dagger}_{i\sigma}\vec{\sigma}_{\sigma\sigma'}C_{i\sigma'}/2$ is the spin operator with $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ as Pauli matrices, $\hat{n}_{i\sigma}=C^{\dagger}_{i\sigma}C_{i\sigma}$, U is the on-site Coulomb repulsion, t is the hopping parameter, and J is the exchange coupling constant. In the Hamiltonian (1), the U term is introduced to partially impose the no-double-occupancy constraint. In the limit $U\rightarrow\infty$, the model is reduced to the t-J model.

To study the Hamiltonian (1) with the Gutzwiller variational approach, we take the trial wave function $|\psi\rangle$ as

$$|\psi\rangle = P_G|\psi_0(\Delta_d,\Delta_{af},\mu)\rangle, \tag{3}$$

where P_G is the Gutzwiller projection operator and it is defined as

$$P_G = \prod_i [1-(1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}], \tag{4}$$

where g is a variational parameter which takes the value between 0 and 1. The choice $g=0$ corresponds to the situation with no doubly occupied sites ($U\rightarrow\infty$), while $g=1$ corresponds to the uncorrelated state ($U=0$). $|\psi_0(\Delta_d,\Delta_{af},\mu)\rangle$ is a Hartree-Fock-type wave function, where Δ_d,Δ_{af},μ are the parameters representing dSC, antiferromagnetism, and chemical potential, respectively. The nature of $|\psi_0\rangle$ depends on the expected long-range behavior. Since it is the purpose of this paper to study the interplay between antiferromagnetism and dSC, we will adopt the wave function which includes both the dSC and antiferromagnetism in a unique variational space.[12,13]

With help of the trial wave function (3), the variational energy $E_{\mathrm{var}}=\langle H\rangle$ is given by

$$E_{\mathrm{var}} = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = NUd + \langle H_t\rangle + \langle H_s\rangle, \tag{5}$$

where

$$\langle H_t\rangle = \frac{\langle\psi|H_t|\psi\rangle}{\langle\psi|\psi\rangle},$$

$$\langle H_s\rangle = \frac{\langle\psi|H_s|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{6}$$

N is the total number of the lattice sites, and $d=\langle n_{i\uparrow}n_{i\downarrow}\rangle$ is the average double occupation number. Obviously, the double occupancy can be modulated by U.

In the calculation of the variational energy, we adopt the Gutzwiller projection method which was formulated originally for the Hubbard Hamiltonian. A clear and simple explanation[24] was given by Ogawa *et al.* and by Vollhardt. In their scheme, the spatial correlations are neglected, and the effect of the projection operator is taken into account by the classical statistical weight factors. In this way, the hopping average and the spin-spin correlation in the state $|\psi\rangle$ are related to those in the state $|\psi_0\rangle$ through the following relations:

$$\frac{\langle\psi|C^{\dagger}_{i\sigma}C_{j\sigma}|\psi\rangle}{\langle\psi|\psi\rangle} = g_t\langle\psi_0|C^{\dagger}_{i\sigma}C_{j\sigma}|\psi_0\rangle,$$

$$\frac{\langle\psi|S_i\cdot S_j|\psi\rangle}{\langle\psi|\psi\rangle} = g_s\langle\psi_0|S_i\cdot S_j|\psi_0\rangle. \tag{7}$$

In the thermodynamic limit, one has the following relation between g and d:[24]

$$g^2 = \frac{d(1-n+d)}{(1-r)(1-w)wr}\frac{(n-2wr)^2}{(n-2d)^2}, \tag{8}$$

and the renormalization factors can be derived as follows:

$$g_t = \frac{n-2d}{n-2rw}\left[\sqrt{\frac{(1-w)(1-n+d)}{1-r}}+\sqrt{\frac{w}{r}}d\right] \times\left[\sqrt{\frac{(1-r)(1-n+d)}{1-w}}+\sqrt{\frac{r}{w}}d\right], \tag{9}$$

$$g_s = \left(\frac{n-2d}{n-2wr}\right)^2. \tag{10}$$

Here n is the average electron number per site. In consideration of the AF order, the square lattice is divided into two sublattices A and B. For sublattice A, we assume $\langle\hat{n}_{i\uparrow}\rangle\equiv r=(n/2)+m$ and $\langle\hat{n}_{i\downarrow}\rangle\equiv w=(n/2)-m$, i.e., a net magnetization $+m$ at each site. For sublattice B, the electron occupation numbers r and w are exchanged, meaning the magnetization $-m$ at each site. Here m represents the AF order parameter in the state $|\psi_0\rangle$. These renormalization factors, g_t and g_s, quantitatively describe the correlation effect of the on-site repulsion. We will comment further on this point below.

In terms of these renormalization factors, the variational energy $E_{\mathrm{var}}=\langle H\rangle$ is rewritten as

$$E_{\mathrm{var}} = \langle H_{\mathrm{eff}}\rangle_0, \tag{11}$$

where H_{eff} is the Gutzwiller renormalized Hamiltonian,

$$H_{\text{eff}} = g_t H_t + g_s H_s + H_U = -g_t t \sum_{i\hat{\eta}\sigma} (C^{\dagger}_{i\sigma} C_{i+\hat{\eta}\sigma} + \text{H.c.}) + g_s J \sum_{i\hat{\eta}} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{\eta}} + NUd. \quad (12)$$

In the mean-field approximation, the renormalized Hamiltonian (12) can be rewritten as

$$H_{\text{MF}} = NUd + \frac{3}{4} N g_s J(\Delta^2 + \chi^2) + 2N g_s J m^2 + \sum_{k\sigma}{}' \{(\epsilon_k - \mu) C^{\dagger}_{k\sigma} C_{k\sigma} + (\epsilon_{k+Q} - \mu) C^{\dagger}_{k+Q\sigma} C_{k+Q\sigma} - \sigma \Delta_{af} (C^{\dagger}_{k\sigma} C_{k+Q\sigma} + C^{\dagger}_{k+Q\sigma} C_{k\sigma})\} - \sum_{k}{}' \Delta_d \eta_k (C_{-k\downarrow} C_{k\uparrow} - C_{-k+Q\downarrow} C_{k+Q\uparrow} + C^{\dagger}_{k\uparrow} C^{\dagger}_{-k\downarrow} - C^{\dagger}_{k+Q\uparrow} C^{\dagger}_{-k+Q\downarrow}), \quad (13)$$

where the electron chemical potential μ has been added, $Q = (\pi, \pi)$ is the commensurate nesting vector, and the prime on the summation symbol indicates that k is limited to half of the original Brillouin zone. In the above equation, we have introduced, respectively, the electron pairing order parameter, the uniform bond order, and the staggered magnetization,

$$\Delta_\eta = \langle C_{i\downarrow} C_{i+\eta\uparrow} - C_{i\uparrow} C_{i+\eta\downarrow} \rangle_0 = \Delta(-\Delta) \text{ when } \eta = x(y), \quad (14)$$

$$\chi_\eta = \chi = \langle C^{\dagger}_{i\uparrow} C_{i+\eta\uparrow} + C^{\dagger}_{i\downarrow} C_{i+\eta\downarrow} \rangle_0, \quad (15)$$

$$m = (-1)^i \langle C^{\dagger}_{i\uparrow} C_{i\uparrow} - C^{\dagger}_{i\downarrow} C_{i\downarrow} \rangle_0 / 2, \quad (16)$$

with $\gamma_k = 2(\cos k_x + \cos k_y)$, $\eta_k = 2(\cos k_x - \cos k_y)$, $\epsilon_k = -(g_t t + \frac{3}{8} g_s J \chi)\gamma_k$, $\Delta_d = \frac{3}{8} g_s J \Delta$, and $\Delta_{af} = 2 g_s J m$. Here the parameter Δ_d is always associated with the factor η_k in Eq. (13), which implies that the superconductivity has a d-wave-like symmetry. The mean-field Hamiltonian (13) is easily diagonalized, giving rise to four bands, $\pm E_{1k}$ and $\pm E_{2k}$, with

$$E_{1k} = \sqrt{(\xi_k - \mu)^2 + (\Delta_d \eta_k)^2},$$

$$E_{2k} = \sqrt{(-\xi_k - \mu)^2 + (\Delta_d \eta_k)^2},$$

$$\xi_k = \sqrt{\epsilon_k^2 + \Delta_{af}^2}. \quad (17)$$

Here $\Delta_d \eta_k$ and Δ_{af} can be regarded, respectively, as the energy gaps associated with the dSC and AF order parameters. The ground-state energy is given by

$$E_{\text{var}}/N = Ud - \mu\delta - \frac{1}{N} \sum_{k}{}' (E_{1k} + E_{2k}) + \frac{3}{4} g_s J(\Delta^2 + \chi^2) + 2 g_s J m^2. \quad (18)$$

By minimizing the ground-state energy, we can obtain the self-consistent equations for the quantities Δ (the electron pairing order parameter), χ, m (staggered magnetization), and d. The chemical potential μ is adjusted to yield the right filling. All the equations are presented as follows:

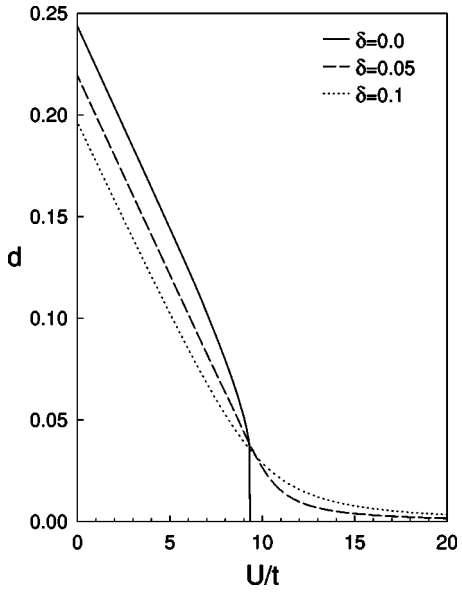

FIG. 1. The average double occupation number d as a function of U at doping $\delta = 0.0$ (solid line), 0.05 (dashed line), and 0.1 (dotted line) for the parameter $t/J = 3.0$ at $T = 0$.

$$\Delta = \frac{1}{4N} \sum_{k}{}' \eta_k^2 \Delta_d \left(\frac{1}{E_{1k}} + \frac{1}{E_{2k}} \right), \quad (19)$$

$$\chi = \frac{1}{4N} \sum_{k}{}' \gamma_k \frac{\epsilon_k}{\xi_k} \left(-\frac{\xi_k - \mu}{E_{1k}} + \frac{-\xi_k - \mu}{E_{2k}} \right), \quad (20)$$

$$m = \frac{1}{2N} \sum_{k}{}' \frac{\Delta_{af}}{\xi_k} \left(\frac{\xi_k - \mu}{E_{1k}} - \frac{-\xi_k - \mu}{E_{2k}} \right) - \frac{1}{4N g_s J} \left(\frac{\partial E_{\text{var}}}{\partial g_t} \frac{\partial g_t}{\partial m} + \frac{\partial E_{\text{var}}}{\partial g_s} \frac{\partial g_s}{\partial m} \right), \quad (21)$$

$$0 = UN + \frac{\partial E_{\text{var}}}{\partial g_t} \frac{\partial g_t}{\partial_d} + \frac{\partial E_{\text{var}}}{\partial g_s} \frac{\partial g_s}{\partial_d}, \quad (22)$$

$$\delta = \frac{1}{N} \sum_{k}{}' \left(\frac{\xi_k - \mu}{E_{1k}} + \frac{-\xi_k - \mu}{E_{2k}} \right). \quad (23)$$

For each doping δ, all the parameters Δ, χ, m, d, and μ are determined self-consistently by Eqs. (19)–(23).

III. RESULTS AND DISCUSSION

Now we summarize our results. First we discuss the average double occupation number d as a function of U. Our calculated results at the doping $\delta = 0.0$ (solid line), 0.05 (dashed line) and 0.1 (dotted line) for the parameter $t/J = 3.0$ at the temperature $T = 0$ are shown in Fig. 1. Hereafter we set $J = 1$. We find that the average double occupation number d at $\delta = 0.0$ decreases linearly as a function of U until $U = 9.3t$, where d drops to zero discontinuously, similar to that reported in Ref. 22. However, we would mention that the recent work by Fleck *et al.* based on the dynamic mean-field

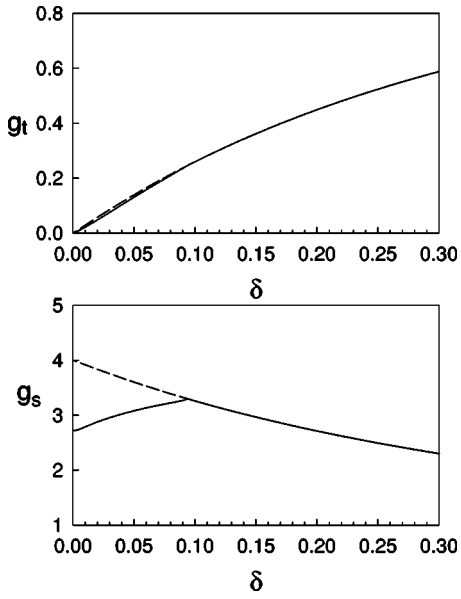

FIG. 2. The Gutzwiller renormalization factors g_t and g_s as functions of doping δ for the parameters $t/J=3.0$ and $U=20t$ at $T=0$ (solid lines). The dashed lines are the corresponding results when the AF order is not considered, i.e., m is fixed to zero.

theory showed that d decreases continuously with increasing U for the half-filled Hubbard model[25]. The origin of this discrepancy is not clear to us, but could be due to the neglecting of the spin fluctuations in our mean-field calculation. For the doped cases, our numerically obtained d as functions of U do not show this discontinuity, and they become flattened and decrease slowly at large U.

The Gutzwiller renormalization factors g_t and g_s as functions of doping δ for the parameters $t/J=3.0$ and $U=20t$ at $T=0$ are shown in Fig. 2. The dashed lines are the corresponding results when the AF order is not considered, i.e., m is fixed to zero. As we mentioned in Sec. II, these factors quantitatively reflect the partially enforced no-double-occupancy constraint due to the on-site Coulomb repulsion U. For large U, the effect of the Gutzwiller renormalization factors is to reduce the kinetic energy and enhance the spin-spin correlation. We find that at low doping, the AF order suppresses the magnitude of g_s while g_t is only slightly affected.

In Fig. 3, we plot the self-consistently obtained order parameters Δ and m as functions of doping δ for the parameters $t/J=3$ and $U=20t$ at $T=0$. The dashed line is the corresponding Δ when the staggered magnetization m is set to zero. It should be noticed that these parameters are the expectation values under the wave function $|\psi_0\rangle$. It is clear that the electron pairing order parameter Δ is drastically suppressed at low doping by the AF order. At half-filling, Δ is reduced to zero and m reaches its maximum value. Near $\delta\sim 0.1$, the AF order vanishes while Δ shows a peak.

We now discuss the dSC order parameter Δ_{SC} and AF order parameter m_{AF} under the wave function $|\psi\rangle$, which are defined as

$$\Delta_{\mathrm{SC}}(\eta)=\langle C_{i\downarrow}C_{i+\eta\uparrow}-C_{i\uparrow}C_{i+\eta\downarrow}\rangle=\Delta_{\mathrm{SC}}(-\Delta_{\mathrm{SC}}) \text{ when } \eta=x(y), \tag{24}$$

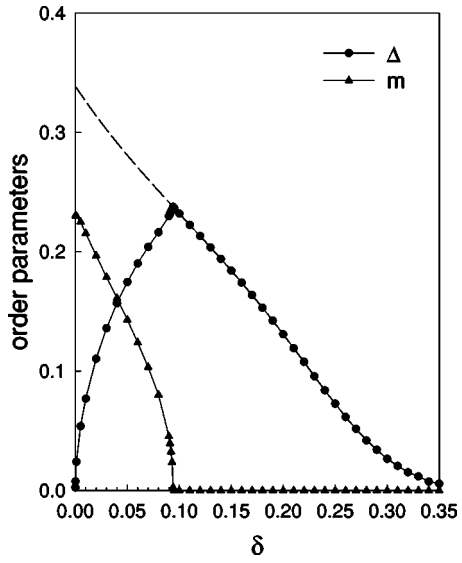

FIG. 3. The self-consistent parameters Δ and m as functions of doping δ for the parameters $t/J=3.0, U=20t$ at $T=0$. The dashed line gives Δ when m is set to zero.

$$m_{\mathrm{AF}}=(-1)^i\langle C_{i\uparrow}^{\dagger}C_{i\uparrow}-C_{i\downarrow}^{\dagger}C_{i\downarrow}\rangle/2. \tag{25}$$

In the Gutzwiller approximation, these parameters are easily obtained from Δ and m with the following renormalization factors:

$$\Delta_{\mathrm{SC}}=g_{\Delta}\Delta,$$

$$m_{\mathrm{AF}}=g_m m. \tag{26}$$

Similar to the derivation of g_t and g_s, we obtain

$$g_{\Delta}=\frac{n-2d}{2(n-2rw)}\left\{\left[\sqrt{\frac{(1-w)(1-n+d)}{1-r}}+\sqrt{\frac{w}{r}d}\right]^2+\left[\sqrt{\frac{(1-r)(1-n+d)}{1-w}}+\sqrt{\frac{r}{w}d}\right]^2\right\}, \tag{27}$$

$$g_m=\frac{n-2d}{n-2wr}. \tag{28}$$

In Fig. 4, we plot the dSC order parameter Δ_{SC}, AF order parameter m_{AF}, and the electron pairing gap (or the RVB order parameter[22]) $\Delta_d=\frac{3}{8}g_sJ\Delta$ as functions of doping δ for $t/J=3.0$ and $U=20t$ at $T=0$. From this phase diagram, we find that the AF and dSC order parameters coexist for a wide doping range, up to $\delta\sim 0.1$, in the ground state. It can also be seen that the AF order parameter is a monotonically decreasing function of δ, but the dSC order parameter shows a non-monotonic dome shape: it increases from zero as the doping increases in the underdoped region and then has a maximum near $\delta\sim 0.15$, after which it decreases to zero at $\delta\sim 0.35$ with increasing doping. Although the present approach applies only at $T=0$, the superconducting transition temperature $T_c(\delta)$ is expected to exhibit a similar δ dependence, and to have a maximum at the optimal doping $\delta\sim 0.15$. It should be noticed that the electron pairing gap Δ_d is also reduced to

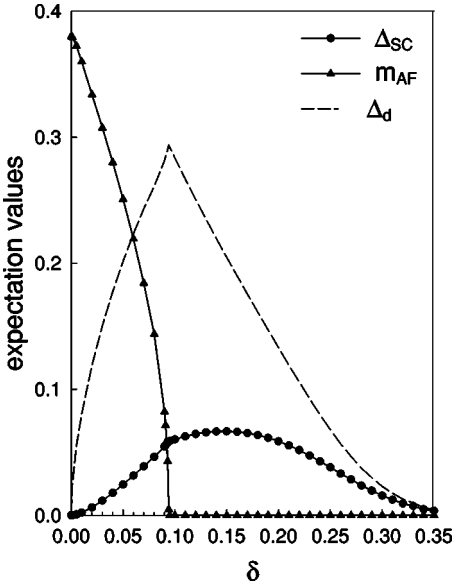

FIG. 4. The dSC order parameter Δ_{SC}, AF order parameter m_{AF}, and the electron pairing gap Δ_d as functions of doping δ for $U=20t$ and $t/J=3.0$ at $T=0$.

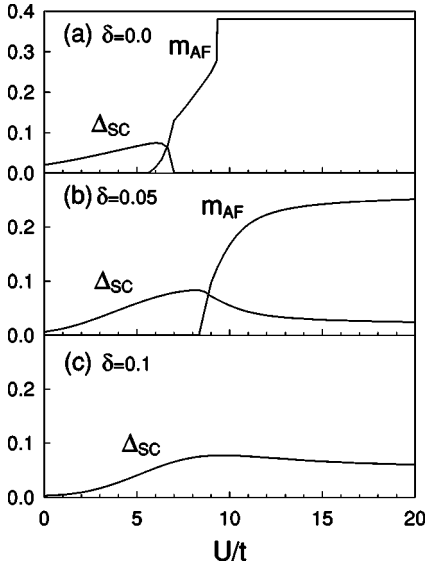

FIG. 6. The dSC and AF order parameters Δ_{SC} and m_{AF} as functions of the Coulomb repulsion U for different dopings with $t/J=3.0$ and $T=0$.

zero at half-filling because of the presence of the AF order. This is quite different from the result in Ref. 22, where the AF order is not considered, and the electron pairing gap increases as the doping decreases.

In order to further understand the effect of the Coulomb repulsion U on the ground-state behavior, calculations for several other values of U are performed. In Fig. 5, we plot the calculated results for $U=5t, 7t, 10t$, and $15t$ with $t/J=3$ and $T=0$. It is clearly seen that with decreasing U, the AF order decreases very quickly with increasing doping, and the coexistent region of the AF and dSC orders is squeezed toward lower doping. Particularly for $U=5t$, the coexistence disappears, and the AF order is completely suppressed by the prevailing dSC order. To illustrate more clearly the dependence of the order parameters on U, we present the parameters Δ_{SC} and m_{AF} as functions of the Coulomb repulsion U for doping $\delta=0.0$ (a), $\delta=0.05$ (b), and $\delta=0.1$ (c) at $T=0$ in Fig. 6. At half-filling [see Fig. 6(a)], for small Coulomb repulsion $U<5.3t$, only the dSC order persists. As U increases up to $U=5.3t$, the AF order begins to show up and coexists with the dSC and the transition appears to be second order. At $U=7t$, there is a discontinuity in the slope of m_{AF} and the dSC order gets completely suppressed by the AF order. For $U>9.3t$, the double occupancy number d drops discontinuously to zero. As a result, the magnitude of m_{AF} jumps from 2.7 to 3.8 and then becomes U-independent. With increasing doping [see Fig. 6(b)], the AF order begins to emerge only at larger U while the dSC order is always in existence. But for doping $\delta \geqslant 0.1$ [see Fig. 6(c)], the AF order completely disappears independent of the magnitude of U.

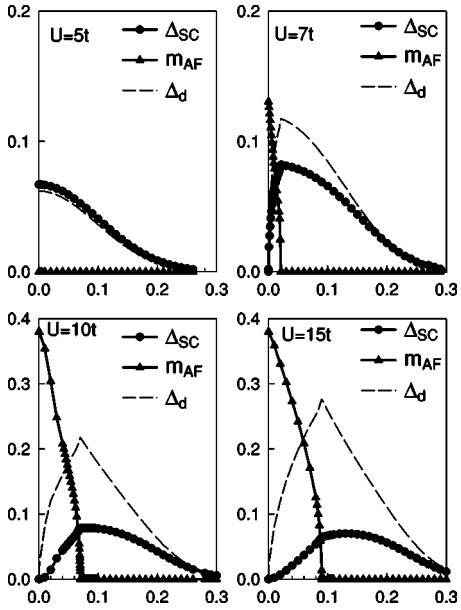

FIG. 5. The dSC order parameter Δ_{SC}, AF order parameter m_{AF}, and the electron pairing gap Δ_d as functions of doping δ for different values of U with $t/J=3.0$ and $T=0$.

With the help of these self-consistent parameters, let us compare the ground-state energy obtained from Eq. (18) with that in Ref. 22 where the contribution from the AF order was neglected. In Fig. 7, we plot our ground-state energy E_{var}/N as a function of doping δ using the parameter $t/J=3.0$ for several different values of U (see the solid lines). The dashed lines here correspond to the results when the contribution from the AF order is not included, i.e., m is fixed to zero.[22] From Fig. 7, we conclude that the ground-state energy with the AF order considered is always lower than that without it.

We now discuss the relevance of our calculations to other theories. Although the t-J model, derived from the large-U Hubbard model, was originally introduced to study the superconductivity based on the RVB theory without AF order,[9,15–18] the inclusion of the AF order based on the same approach was done at a much later stage. In all these studies, the no-double-occupancy constraint has been globally en-

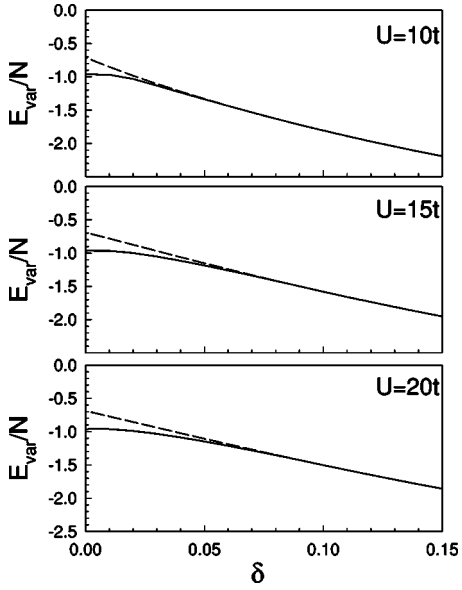

FIG. 7. Doping dependence of the ground-state energy for several different U for $t/J=3.0$. The dashed lines are the corresponding results when the AF order is not considered, i.e., m is fixed to zero.

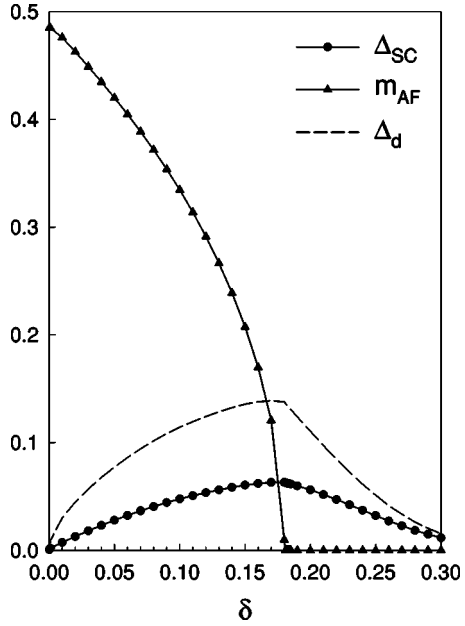

FIG. 8. The dSC order parameter Δ_{SC}, AF order parameter m_{AF}, and the electron pairing gap Δ_d as functions of doping δ for $U=15t$ and $t/J=3.0$ at $T=0$. Here the derivatives of g_t and g_s with m in the self-consistent equations are neglected.

forced. By use of the *t-J* or similar models, several groups have investigated the interplay between the AF and dSC orders with somewhat different mean-field approximations from ours.[19,20,26–29] While the double occupancy is completely excluded from the standard *t-J* model, our current *t-J-U* model with finite U allows the partial double occupation so that we can understand the subtle effect due to the electron-electron correlation. For small U, our results show that only the dSC order exists in the ground state, which describes the physics of the "gossamer superconductor." In the limit of infinite U, the *t-J-U* model is reduced to the *t-J* model. In this case, our phase diagrams show that the AF and dSC orders coexist with each other from small δ up to $\delta\sim 0.1$, and after that the AF order completely disappears. This feature is in good agreement with the VMC results for the *t-J* model.[12–14] At the same time, we notice that the coexistence between the AF and dSC orders persists up to optimal doping $\delta\sim 0.15$ in the slave-boson scheme.[19,20] We would like to mention that a similar large coexistence can be obtained if we neglect the derivatives of g_t and g_s with m in our derivation of the self-consistent equations, i.e., replace Eq. (21) with the following one:

$$m=\frac{1}{2N}\sum_k{}'\frac{\Delta_{af}}{\xi_k}\left(\frac{\xi_k-\mu}{E_{1k}}-\frac{-\xi_k-\mu}{E_{2k}}\right). \tag{29}$$

In this way, we can perform similar calculations as above. In Fig. 8, we present such a phase diagram with $t/J=3.0$ and $U=15t$ at $T=0$. It can be seen that in this case, the AF and dSC orders coexist up to doping $\delta\sim 0.18$. However, if one uses $t/J=4.0$ and $U=15t$, the coexistent region is pushed downward to doping $\delta\sim 0.15$, which is consistent with the slave-boson result. But such a large coexistent region seems not to be favored by the experimental and simulation results. Moreover, based on this approximation, the system at half-filling would always be an AF insulator, independent of the magnitude of U. This is in strong contrast to what has been obtained from our current approach based on minimizing the total energy of the system.

So far the experimental evidence for the coexistence of the AF and dSC orders in cuprate superconductors seems inconclusive. For example, the long-range AF order observed in the insulating $La_{2-x}Sr_xCuO_4$ is sensitive to doping,[1] which disappears rapidly at $x\sim 0.03$. But there also existed several experimental results which appeared to indicate the coexistence of antiferromagnetism and superconductivity over a wide doping range in cuprate superconductors.[2–8] Especially, the AF order was claimed to have been observed in underdoped $YBa_2Cu_3O_{6.5}$ and $YBa_2Cu_3O_{6.6}$ superconductors by neutron-scattering experiments from different groups.[6,8] It is apparent that more experiments are needed to confirm the coexistence of the long-range AF order with the dSC state in HTS.

IV. SUMMARY

In summary, we have studied the coexistence of the antiferromagnetism and dSC in a renormalized mean-field theory based on the Gutzwiller approximation for a two-dimensional *t-J-U* model. The role of the Hubbard interaction U is to partially enforce the no-double-occupancy constraint, and it provides us with a better understanding of the subtle effect due to the electron-electron correlation. Our results show that the AF and dSC orders coexist below the doping $\delta\sim 0.1$ at large U with $t/J=3.0$. And we find that the coexisting state has a lower ground-state energy than that of a pure dSC state. The dSC order increases from zero as doping increases in the underdoped regime and reaches a maxi-

mum near the optimal doping $\delta \sim 0.15$, after which it decreases to zero at $\delta \sim 0.35$ with increasing doping. With decreasing U, the coexistent region is squeezed toward low doping. There is no coexistence between AF and dSC orders for small U ($<5.3t$), where the AF order is completely suppressed and the "gossamer superconductivity" is found even at half-filling. For the large U, our system at half-filling is always an AF insulator in which both the electron pairing gap and the dSC order parameter are suppressed to zero. Our result at large U should correspond to the physical regime. The reason why the existence of the long-range AF order has not been firmly confirmed by experiments in the underdoped HTS is probably due to the neglecting of the AF fluctuations in the mean-field approximation. It is believed that the effect of the AF fluctuations may break the long-range AF order into short-range orders, and this conjecture needs to be examined more carefully in future theories and experiments on cuprate superconductors.

Finally, we would like to mention that in addition to the AF and dSC orders considered here, there are other competing orders such as stripe and flux state, in the underdoped region of cuprate superconductors.[30,31] It has been found that at zero temperature, the flux state is unstable in the t-J model, but it may show up at finite temperature, or in the vortex cores if J is chosen to be larger than $0.5t$.[31] In our present mean-field theory, which is valid only at zero temperature, the obtained order parameters for the dSC and the staggered magnetization are spatially uniform. To seek the inhomogeneous solutions such as stripe phases for these order parameters, we need to use the variational Monte Carlo method, or the Bogoliubov–de Gennes equations, and that will be a topic for future study.

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