Study of gossamer superconductivity and antiferromagnetism in the $t$-$J$-$U$ model

Feng Yuan$^{1,2}$, Qingshan Yuan$^{1,3}$, C. S. Ting$^1$, and T. K. Lee$^4$

$^1$ Texas Center for Superconductivity and Advanced Materials and Department of Physics, University of Houston, Houston, TX 77204

$^2$ Department of Physics, Qingdao University, Qingdao 266071, China

$^3$ Pohi Institute of Solid State Physics, Tongji University, Shanghai 200092, China

$^4$ Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan 11529

(March 23, 2022)

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 $\delta$ 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 $U$ increased to a critical value, the AF order shows up and coexists with the dSC in the underdoped regime. 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.

PACS: 74.25.Jb, 71.10.Fd, 74.72.-h, 74.25.Ha

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$_2$Cu$_3$O$_{6.5}$, providing the 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$^{15-18}$, 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 that 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 low doping regime until it disappears for $U < 5.3t$, where the "gossamer superconductivity" is found even at half
II. THEORETICAL FRAMEWORK

We start from the $t$-$J$-$U$ model on a square lattice:

$$H = H_t + H_s + H_U,$$

(1)

with

$$H_t = -t \sum_{i,j} (C_{i\sigma}^\dagger C_{j+\hat{i}\sigma} + \text{h.c.}),$$

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

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

(2)

where $\hat{n}_i = \hat{x}$ and $\hat{y}$, $C_{i\sigma}^\dagger$ ($C_{i\sigma}$) is the electron creation (annihilation) operator, $\mathbf{S}_i = \sum_{\sigma} \hat{C}_{i\sigma}^\dagger \sigma_{\sigma\sigma} C_{i\sigma}/2$ is the spin operator with $\sigma = (x, y, z)$ as Pauli matrices, $\hat{n}_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$, $U$ 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

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

(3)

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

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

(4)

here $g$ 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 $\Delta_d, \Delta_{af}, \mu$ 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.

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

$$E_{\text{var}} = \frac{\langle \psi \mid H \mid \psi \rangle}{\langle \psi \mid \psi \rangle} = NUd + \langle H_t \rangle + \langle H_s \rangle,$$

(5)

where

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

$$\langle H_s \rangle = \frac{\langle \psi \mid H_s \mid \psi \rangle}{\langle \psi \mid \psi \rangle},$$

(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 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

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

$$\frac{\langle \psi \mid S_i \cdot S_j \mid \psi \rangle}{\langle \psi \mid \psi \rangle} = g_s \langle \psi_0 \mid S_i \cdot S_j \mid \psi_0 \rangle.$$

(7)

In the thermodynamic limit, one has

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

(8)

and the renormalization factors can be derived to have the following expressions,

$$g_t = \frac{n-2d}{n-2wr} \left[ \sqrt{\frac{(1-w)(1-n+d)}{1-r}} + \frac{w}{r} \right]$$

$$\times \left[ \sqrt{\frac{(1-r)(1-n+d)}{1-w}} + \frac{r}{w} \right],$$

(9)

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

(10)

Here $n$ is the average electron number per site. In order to consider the AF order, the square lattice is divided into two sublattices $A$ and $B$. For sublattice $A$ we assume $\langle \hat{n}_{i\uparrow} \rangle = r = \frac{1}{2} + m$ and $\langle \hat{n}_{i\downarrow} \rangle = w = \frac{1}{2} - m$, 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 further comment on this point below.

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

\[
E_{\text{var}} = \langle H_{\text{eff}} \rangle_0,
\]

where \( H_{\text{eff}} \) is the Gutzwiller renormalized Hamiltonian:

\[
H_{\text{eff}} = g_t H_t + g_s H_s + H_U
\]

\[
= -g_t \sum_{ij} (C^\dagger_{i\sigma} C_{i+ij\sigma} + \text{h.c.})
+ g_s \sum_{i} s_i \cdot s_{i+\hat{q}} + N Ud.
\]

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

\[
H_{MF} = N Ud + \frac{3}{4} N g_s J (\Delta^2 + \chi^2) + 2 N g_s J m^2
+ \sum_{k\sigma} \left\{ (\epsilon_k - \mu) C^\dagger_{k\sigma} C_{k\sigma} + (\epsilon_{k+Q} - \mu) C^\dagger_{k+Q\sigma} C_{k+Q\sigma} \right\}
- \sigma \Delta_{af} (C^\dagger_{k\sigma} C_{k+Q\sigma} + C^\dagger_{k+Q\sigma} C_{k\sigma})
- \sum_k \Delta_d \eta_k (C_{-k\uparrow} C_{k\uparrow} - C_{-k+Q\uparrow} C_{k+Q\uparrow})
+ C^\dagger_{k\uparrow} C_{-k\downarrow} - C^\dagger_{k+Q\uparrow} C_{k+Q\downarrow},
\]

where the electron chemical potential \( \mu \) 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 Brillouin zone. In the above equation, we have introduced respectively the electron pairing order parameter, the hopping average and the staggered magnetization

\[
\Delta_\eta = \langle C^\dagger_{i\downarrow} C_{i+\eta \uparrow} - C^\dagger_{i\uparrow} C_{i+\eta \downarrow} \rangle_0
= \Delta + (-\Delta) \text{ when } \eta = x (y),
\]

\[
\chi_\eta = \chi = \langle C^\dagger_{i\uparrow} C_{i+\eta \uparrow} + C^\dagger_{i\downarrow} C_{i+\eta \downarrow} \rangle_0,
\]

\[
m = (-1)^i \langle C^\dagger_{i\uparrow} C_{i-\eta \uparrow} - C^\dagger_{i\downarrow} C_{i-\eta \downarrow} \rangle_0/2,
\]

with \( \gamma_k = 2(\cos k_x + \cos k_y), \quad \eta_k = 2(\cos k_x - \cos k_y), \quad \epsilon_k = -(g_t + \frac{3}{2} g_s J \chi) \gamma_k, \Delta_d = \frac{1}{2} g_s J \Delta, \text{ and } \Delta_{af} = g_s J m. \)

Here the parameter \( \Delta_\eta \) is always associated with the factor \( \eta_k \) 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

\[
E_{1k} = \sqrt{\left( \xi_k - \mu \right)^2 + \left( \Delta_d \eta_k \right)^2},
E_{2k} = \sqrt{\left( -\xi_k - \mu \right)^2 + \left( \Delta_d \eta_k \right)^2},
\]

\[
\xi_k = \sqrt{\epsilon_k^2 + \Delta_{af}^2}.
\]

Here \( \Delta_d \eta_k \) and \( \Delta_{af} \) can be regarded respectively as the energy gap associated with the dSC and the AF order parameter. The ground state energy is given by

\[
E_{\text{var}}/N = Ud - \mu \delta - \frac{1}{N} \sum_k (E_{1k} + E_{2k})
+ \frac{3}{4} g_s J (\Delta^2 + \chi^2) + 2 g_s J m^2.
\]

By minimizing the ground state energy, we can obtain the self-consistent equations for the quantities \( \Delta \) (the electron pairing order parameter), \( \chi \), \( m \) (staggered magnetization), \( d \) and the chemical potential \( \mu \) as follows

\[
\Delta = \frac{1}{4N} \sum_k \eta_k^2 \Delta_d (\frac{1}{E_{1k}} + \frac{1}{E_{2k}}),
\]

\[
\chi = \frac{1}{4N} \sum_k \eta_k^2 \xi_k (\frac{-\xi_k - \mu}{E_{1k}} + \frac{\xi_k - \mu}{E_{2k}}),
\]

\[
m = \frac{1}{2N} \sum_k \Delta_{af} \eta_k \xi_k \left( \frac{E_{1k}}{E_{1k}} - \frac{E_{2k}}{E_{2k}} \right),
\]

\[
\delta = \frac{1}{N} \sum_k \left( \frac{\xi_k - \mu}{E_{1k}} - \frac{\xi_k - \mu}{E_{2k}} \right).
\]

For each doping \( \delta \), all the parameters \( \Delta, \chi, m, d \) and \( \mu \) are determined self-consistently by the Eqs. (19)-(23).

III. RESULTS AND DISCUSSION

Now we summarize our results. Firstly 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. We find that the average double occupation number \( d \) at \( \delta = 0.0 \) decreases linearly as function of \( U \) till \( U = 9.3t \), where \( d \) shows the similar behavior of discontinuity as reported in Ref. [22]. But 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 \( \delta \) 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 or \( m \) 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 projector operators 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.
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 $T=0$.

FIG. 2. The Gutzwiller renormalization factors $g_t$ and $g_s$ as functions of doping $\delta$ 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.

In Fig. 3, we plot the self-consistently obtained order parameters $\Delta$ and $m$ as functions of doping $\delta$ for the parameters $t/J = 3.0$, $U = 20t$ at $T = 0$. The dashed line is the $\Delta$ with $m$ is set to zero.

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

$$\Delta_{SC}(\eta) = (C_{i+\eta}^\dagger C_i - C_i^\dagger C_{i+\eta})$$
$$= \Delta_{SC} (-\Delta_{SC}) \text{ when } \eta = x (y),$$

$$m_{AF} = (-1)^i(C_{i+\eta}^\dagger C_i^\dagger - C_i^\dagger C_{i+\eta})/2.$$  

(24)  

(25)

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

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

$$m_{AF} = g_m m.$$  

(26)

Similar to the method of deriving $g_t$ and $g_s$, we obtain

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

(27)

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

(28)

In Fig. 4 we plot the dSC order parameter $\Delta_{SC}$, AF order parameter $m_{AF}$ and the electron pairing gap (or the RVB order parameter) $\Delta_d = \frac{1}{2}g_s J\Delta$ as functions of doping $\delta$ 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

the AF order. At half filling, $\Delta$ is reduced to zero and $m$ reaches to its maximum value. Near $\delta \sim 0.1$, the AF order vanishes while $\Delta$ shows a peak.
\( \delta \sim 0.1 \), in the ground state. It can also be seen that the AF order parameter is a monotonically decreasing function of \( \delta \), 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 \( \delta \) dependence, and to have a maximum at the optimal doping \( \delta \sim 0.15 \). It should be noticed that the electron pairing gap \( \Delta_d \) is also reduced to zero at half filling because of the presence of the AF order. This is quite different from the case in Ref. [22], where the AF order is not considered, and the electron pairing gap increases as the doping decreases.

![Graph](image)

**FIG. 4.** The dSC order parameter \( \Delta_{SC} \), AF order parameter \( m_{AF} \) and the electron pairing gap \( \Delta_d \) as functions of doping \( \delta \) for \( U = 20t \) and \( t/J = 3.0 \) at \( T = 0 \).

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 \( \Delta_{SC} \) 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 a 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 at \( U > 7t \) where our system becomes an AF insulator. 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 becomes \( U \) independent for large \( U \). And with increasing doping (see Fig. 6(b)), the AF order exists only for larger \( U \) while the dSC order is always in presence. But for doping \( \delta \geq 0.1 \) (see Fig. 6(c)), the AF order completely disappears independent of the magnitude of \( U \).

![Graph](image)

**FIG. 5.** The dSC order parameter \( \Delta_{SC} \), AF order parameter \( m_{AF} \) and the electron pairing gap \( \Delta_d \) as functions of doping \( \delta \) for different values of \( U \) with \( t/J = 3.0 \) and \( T = 0 \).

![Graph](image)

**FIG. 6.** The dSC and AF order parameters \( \Delta_{SC} \) and \( m_{AF} \) as functions of the Coulomb repulsion \( U \) for different dopings 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 of Ref. [22] in which the contribution from the AF order was neglected. In Fig.7, we plot our ground state energy \( E_{\text{var}}/N \) as a function of doping \( \delta \) 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. From Fig.7, we conclude that the ground state energy with the AF order considered is always lower than that without it.

![Graph showing doping dependence of the ground state energy](image)

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

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 enforced. Using the \( t\)-\( J \) or a similar model and based upon other type of mean field approximations, there exist several works\(^{19,20,25-28} \) investigating the existence of both AF and dSC orders in the system. While the double occupancy is globally excluded from the standard \( t\)-\( J \) model, our current \( t\)-\( J \)-\( U \) model with finite \( U \) allows partial enforcement of the no double occupancy constraint, and to understand the subtle effect due to the electron-electron correlation. For the case of 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 \( \delta \) 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 mention that the 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,

\[
m = \frac{1}{2N} \sum_k \frac{\Delta_{af}(\xi_k - \mu)}{E_{1k}} = \frac{-\xi_k - \mu}{E_{2k}}.
\]

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 \( \delta \sim 0.18 \). But it seems that such a large coexistent region is not 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 contrary to what has been obtained from our current approach based on minimizing the total energy of our system.

![Graph showing phase diagram](image)

**FIG. 8.** The dSC order parameter \( \Delta_{SC} \), AF order parameter \( m_{AF} \) and the electron pairing gap \( \Delta_d \) as functions of doping \( \delta \) 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.

So far the experimental evidences for the coexistence of the AF and dSC orders in cuprate superconductors seem not conclusive. For example, the long range AF order observed in the insulating La\(_{2-x}\)Sr\(_x\)CuO\(_4\) 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$_2$Cu$_3$O$_{6.5}$ and YBa$_2$Cu$_3$O$_{6.6}$ 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 maximum 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.

ACKNOWLEDGMENTS

The authors would like to thank Prof. S. P. Feng, J. H. Qin, J. Y. Gan, and H. Y. Chen for the helpful discussions. This work was supported by the Texas Center for Superconductivity and Advanced Materials at the University of Houston, and by a grant from the Robert A. Welch Foundation.

1 For reviews, see D. J. Scalapino, Phys. Rep. 250, 329(1995).
2 A. Weidinger, Ch. Niedermayer, A. Golnik, R. Simon, E. Recknagel, J. I. Budnick, B. Chamberland, and C. Baines, Phys. Rev. Lett. 62, 102 (1989).
3 R. F. Kiefl, J. H. Brewer, J. Carolan, P. Dosanjh, W. N. Hardy, R. Kadono, J. R. Kempton, R. Krahn, P. Schleger, B. X. Yang, Hu Zhou, G. M. Luke, B. Sternlieb, Y. J. Uemura, W. J. Kossler, X. H. Yu, E. J. Ansaldo, H. Takagi, S. Uchida, and C. L. Seaman, Phys. Rev. Lett. 63, 2136 (1989).
4 T. Suzuki, T. Goto, K. Chiba, T. Shinoda, T. Fukase, H. Kimura, K. Yamada, M. Ohashi and Y. Yamaguchi, Phys. Rev. B 57, 3229 (1998).
5 H. Kimura, K. Hirota, H. Matsushita, K. Yamada, Y. Endoh, S.-H. Lee, C. F. Majkrzak, R. Erwin, G. Shirane, M. Groven, Y. S. Lee, M. A. Kastner and R. J. Birgeneau, Phys. Rev. B 59, 6517 (1999).
6 Y. Sidis, C. Ulrich, P. Bourges, C. Bernhard, C. Niedermayer, L. P. Regnault, N. H. Anderson and B. Keimer, Phys. Rev. Lett. 86, 4100 (2001).
7 J. A. Hodges, Y. Sidis, P. Bourges, I. Mirebeau, M. Hennion, and X. Chaud, Phys. Rev. B 66, R020501(2002).
8 H. A. Mook, P. Dai, S. M. Hayden, A. Hiess, J. W. Lynn, S.-H. Lee, and F. Dojan, Phys. Rev. B 66, 144513(2002).
9 P. W. Anderson, Science 235, 1196 (1987).
10 F. C. Zhang and T. M. Rice, Phys. Rev. B 37, 3759 (1988).
11 G. J. Chen, R. Joynt, F. C. Zhang and C. Gros, Phys. Rev. B 42, 2662 (1990).
12 T. Giamarchi and C. Lhuillier, Phys. Rev. B 43, 12943(1991).
13 A. Himeda and M. Ogata, Phys. Rev. B 60, R9935(1999).
14 C. T. Shih, Y. C. Chen, C. P. Chou, and T. K. Lee, cond-mat/0408422 (2004).
15 G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 63, 973(1987).
16 G. Kotliar, Phys. Rev. B 37, 3664(1988); G. Kotliar and J. Liu, ibid. 38, 5142(1988).
17 Z. Zou and P. W. Anderson, Phys. Rev. B 37, 627(1988).
18 Y. Suzumura, Y. Hasegawa and H. Fukuyama, J. Phys. Soc. Jpn. 57, 401(1988).
19 M. Inaba, H. Matsukawa, M. Saitoh and H. Fukuyama, Physica C 257, 299(1996).
20 H. Yamase and H. Kohno, Phys. Rev. B 69, 104526(2004).
21 R. B. Laughlin, cond-mat/0209269 (2002).
22 F. C. Zhang, Phys. Rev. Lett. 90, 207002(2003); J. Y. Gan, F. C. Zhang, and Z. B. Su, cond-mat/0308398 (2003).
23 M. C. Gutzwiller, Phys. Rev. Lett. 10, 159(1963); Phys. Rev. A 134, 923(1964); ibid. 137, 1726(1965).
24 T. Ogawa, K. Kanda, and T. Matsubara, Prog. Theor. Phys. 53, 614(1975); D. Vollhardt, Rev. Mod. Phys. 56, 99(1984).
25 M. Inui, S. Doniach, P. J. Hirschfeld, and A. E. Ruckenstein, Phys. Rev. B 37, R2320(1988).
26 B. Kyung, Phys. Rev. B 62, 9083(2000).
27 A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B 62, R9238(2000).
28 M. Ogata and A. Himeda, J. Phys. Soc. Jpn. 72, 374(2003).
29 A. Himeda, T. Kato, and M. Ogata, Phys. Rev. Lett. 88, 117001 (2002).