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Cooperative behavior of RVB, flux phase, and antiferromagnetic states

H.L. Chiueh, D.S. Chuu¹

Department of Electrophysics, National Chiao Tung University, Hsinchu, Taiwan, ROC

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Abstract

The coexistence of RVB, flux phase, and antiferromagnetic states for the t - J model is studied within the frame work of the mean-field theory by means of the slave-boson approach. Two simple relations among these three order parameters manifesting the cooperative behavior of these states are derived. A phase diagram separating the antiferromagnetic from the non-antiferromagnetic state is obtained. Comparison with available previous work shows that our result agrees reasonably well. © 1997 Elsevier Science B.V.

Keywords: Antiferromagnetic order; Holons; Phase diagram; RVB model; Spinons

Although few exact results were attained after Hubbard's original work, it was believed that Hubbard's model could yield rich phases as temperature, doping, and the parameter t/U were changed. The model attracted lots of attention again when high temperature superconductors (HTSC) were discovered. Afterwards, various numerical calculations have been performed for the 1D and 2D Hubbard (and t - J) models.

For the 1D system, many interesting phases, such as phase separation [1], were obtained as the parameters were changed. For the 2D system, a phase separated region was also observed [2]. From the results of numerical works it was conjectured that superconducting instability might occur in the neighborhood of phase separation [3], which lies along the line going from low doping, large t/J , to large doping, small t/J .

Although some numerical results also indicated that there is no superconducting phase for the t - J model

when the doping concentration is non-zero [4], it does not, however, mean that the superconducting phase should be ruled out when the model is modified. For example, Anderson [5,6] argued that an increasing quantum fluctuation, such as including the next nearest hopping or phonon effect, would make the antiferromagnetic state unstable and the resonance valence bond (RVB) state would stabilize it. For this reason, various mean-field ground states, such as the π -flux phase [7], the staggered flux phase [8], the commensurate flux phase [9], and the uniform flux phase [10], have been proposed to explain the unusual properties of HTSC.

The above-mentioned mean-field states are not independent from each other. It is found that, at half filling, the π -flux phase (commensurate flux phase), the $s + id$ -wave RVB state [11], and the state of d -wave RVB coexisting with π -flux phase [12] are all equivalent by a local $SU(2)$ transformation. Lieb [13] also proved exactly that, among the various flux phases,

¹ Corresponding author.

the π -flux phase is the one with the lowest energy. Recently, Wen and Lee [14] proposed a $SU(2)$ mean-field theory to emphasize the local $SU(2)$ symmetry and to explain the properties in the under-doped region. But all these states are unstable in contrast with the antiferromagnetic ground state at half filling, which was not taken into account in their work.

Among these slave-boson based mean-field theories attentions have been directed to the competition between various flux states and RVB state, but these states do not yield good magnetic properties near half filling. Although these theories obtained plausible success to explain the properties in the superconducting and strange-metal region, they failed in the antiferromagnetic region. With the expectation of being a unified theory, the inclusion of the Néel order is needed to connect the antiferromagnetic phase smoothly to the other phases. Recently, Inaba et al. [15] have considered these three orders together in the frame work of the mean-field theory with an approach different from ours which will be described below.

Although the slave-fermion based mean-field theories [16] could explain various magnetic properties, they seemed to be unable to make good progress beyond that region. In this work, we will investigate the relationship between the Néel state, staggered flux, and the spin singlet state for the t - J model by using the slave-boson technique.

The Hamiltonian is written as

$$\begin{aligned}
 H = & -t \sum_{(i,j),\sigma} (f_{i\sigma}^+ f_{j\sigma} b_j^+ b_i + \text{h.c.}) \\
 & + J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \cdot \hat{n}_j \right) \\
 & - \mu \sum_i \hat{n}_i - i \sum_i a_i (\hat{n}_i + \hat{n}_i^b - 1). \quad (1)
 \end{aligned}$$

In the above expression, the electron operator $c_{i\sigma}$ has been decomposed as $c_{i\sigma} = f_{i\sigma} b_i^+$, where $f_{i\sigma}$ is the fermionic (spinon) operator, and b_i is the hard core bosonic (holon) operator. These operators satisfy the single occupancy constraint $\sum_{\sigma} f_{i\sigma}^+ f_{i\sigma} + b_i^+ b_i = 1$ at each site and the Lagrangian multiplier a_i is introduced to fulfill that constraint. The J term in Eq. (1) should be expressed in the electronic operator representation, but it can also be represented by spinon operators without employing any approxima-

tion under the single occupancy constraint, namely $\vec{S}_i = (1/2) \sum_{\alpha\beta} f_{i\alpha}^+ \vec{\sigma}_{\alpha\beta} f_{i\beta}$, and $\hat{n}_i = \sum_{\sigma} f_{i\sigma}^+ f_{i\sigma}$ in Eq. (1). Because of the operator identities

$$\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \cdot \hat{n}_j = -\frac{1}{2} \hat{\Delta}_{ij}^+ \hat{\Delta}_{ij}$$

and

$$\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \cdot \hat{n}_j = -\frac{1}{2} (\hat{\chi}_{ij} \hat{\chi}_{ji} + \hat{n}_i \cdot \hat{n}_j - \hat{n}_i),$$

where

$$\hat{\Delta}_{ij}^+ = f_{i\uparrow}^+ f_{j\downarrow}^+ - f_{i\downarrow}^+ f_{j\uparrow}^+ = \hat{\Delta}_{ji}^+, \quad \hat{\Delta}_{ij} = (\hat{\Delta}_{ij}^+)^+,$$

and $\hat{\chi}_{ij} = \sum_{\sigma} f_{i\sigma}^+ f_{j\sigma}$, one gets

$$\begin{aligned}
 \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \cdot \hat{n}_j = & -\frac{\gamma_1^2}{2} \hat{\Delta}_{ij}^+ \hat{\Delta}_{ij} \\
 & -\frac{\gamma_2^2}{2} (\hat{\chi}_{ij} \hat{\chi}_{ji} + \hat{n}_i \cdot \hat{n}_j - \hat{n}_i) \\
 & + \gamma_3^2 \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \cdot \hat{n}_j \right), \quad (2)
 \end{aligned}$$

with $\gamma_1^2 + \gamma_2^2 + \gamma_3^2 = 1$. In what follows, we will apply the Hubbard–Stratonovich (HS) transformation for the γ_1 , γ_2 , and γ_3 terms. It will then reproduce the spin singlet order parameter (RVB) $\Delta_{ij}^{0*} = \langle f_{i\uparrow}^+ f_{j\downarrow}^+ - f_{i\downarrow}^+ f_{j\uparrow}^+ \rangle$, the particle–hole channel order parameter $\chi_{ij}^0 = \langle \sum_{\sigma} f_{i\sigma}^+ f_{j\sigma} \rangle$, and the antiferromagnetic order parameter $S_{ij}^z = \langle S_i^z - S_j^z \rangle$, respectively.

In the usual Hartree–Fock approximation, $\gamma_1^2 = \gamma_2^2 = \gamma_3^2 = 1$ is used with the assumption that these three order parameters contribute to the mean-field Hamiltonian equivalently in different ranges of momentum space. As will be shown later, this is not true in the present case. With the HS transformation method we used here no such assumption is needed. Furthermore, one is able to know how significantly these three order parameters contribute to the dynamics of Hamiltonian by observing the γ values. For example, for larger γ_1 , the order parameter Δ_{ij}^{0*} will affect the dynamics more significantly. Besides, by observing the γ values, we could study how significant the quantum fluctuation is by these three order parameters. Again, for $\gamma_1 \neq 0$, even if $\Delta_{ij}^{0*} = 0$, the quantum fluctuation produced by the order parameter Δ_{ij}^{0*} still exists and the fluctuation is more significant when γ_1 is larger. Therefore, it is interesting to ask what will be the appropriate

values for the γ 's? In the conventional approaches, the γ 's were chosen to be $(\gamma_1^2, \gamma_2^2, \gamma_3^2) = (1, 0, 0)$ [6,12], $(\gamma_1^2, \gamma_2^2, \gamma_3^2) = (3/4, 3/4, -1/2)$ [8,17] or $(\gamma_1^2, \gamma_2^2, \gamma_3^2) = (0, 1/2, 1/2)$ [18]. Usually, one could not give good reasons to explain why these γ 's have to be chosen in that way except for the second case by Lee et al. Lee decomposed these three terms by expressing them as sums of some components. They required the components contained in the sum of any two terms were excluded from components contained in the other term. Such kind of choice is not suitable for the discussion of antiferromagnetic order. In fact $\gamma_2^2 = -1/2$ corresponds to the case of ferromagnetic order rather than antiferromagnetic order, so one has to choose zero magnetic moment at each site [8] to avoid this difficulty. In our study we treat the γ parameters as free parameters and minimize the free energy with respect to them to obtain suitable values for γ . The minimization of the free energy results two simple closed expressions among the order parameters Δ_{ij}^0 , χ_{ij}^0 and $S_{ij}^{\alpha,0}$. From these two expressions, one can find that a cooperative behavior between them exists, instead of competition of these order parameters. To see this, let us rewrite the Hamiltonian in Eq. (1) as

$$\begin{aligned}
H = & -\frac{\gamma_1^2}{2} J \sum_{\langle ij \rangle} \widehat{\Delta}_{ij}^+ \widehat{\Delta}_{ij} - \frac{\gamma_2^2}{2} J \sum_{\langle ij \rangle} \widehat{\chi}_{ij} \widehat{\chi}_{ji} \\
& - \frac{\gamma_3^2}{2} J \sum_{\langle ij \rangle} \left\{ \left(\widehat{S}_i - \widehat{S}_j \right)^2 \right. \\
& \left. - \frac{3}{4} \left[\widehat{n}_i \left(1 - \widehat{n}_{i\uparrow} \widehat{n}_{i\downarrow} \right) + \widehat{n}_j \left(1 - \widehat{n}_{j\uparrow} \widehat{n}_{j\downarrow} \right) \right] \right\} \\
& - \frac{(2\gamma_2^2 + \gamma_3^2)}{4} J \sum_{\langle ij \rangle} \widehat{n}_i \widehat{n}_j - (\mu - \gamma_2^2 J) \sum_i \widehat{n}_i \\
& - t \sum_{\langle ij \rangle} \left(\widehat{\chi}_{ij} \widehat{G}_{ji} + \text{h.c.} \right) - i \sum_i a_i \left(\widehat{n}_i + \widehat{n}_i^b - 1 \right),
\end{aligned} \tag{3}$$

where $\widehat{G}_{ji} = b_j^\dagger b_i$. Now, make the HS transformation for the three γ terms by multiplying "1" in each τ -slice into the functional integral of Lagrangian:

$$\begin{aligned}
1 = & \frac{1}{2} \int \frac{d\Delta_{ij}^* d\Delta_{ij}}{2\pi i} \exp \left[-\frac{1}{2} \left(\Delta_{ij}^* - \gamma_1 \widehat{\Delta}_{ij}^+ \right) (\text{c.c.}) \right] \\
= & \frac{1}{2} \int \frac{d\chi_{ij}^* d\chi_{ij}}{2\pi i} \exp \left[-\frac{1}{2} \left(\chi_{ij} - \gamma_2 \widehat{\chi}_{ij} \right) (\text{c.c.}) \right]
\end{aligned}$$

$$= \frac{1}{2} \int \frac{dS_{ij}^\alpha}{\sqrt{\pi}} \exp \left\{ -\frac{1}{2} \left[S_{ij}^\alpha - \gamma_3 \left(\widehat{S}_i^\alpha - \widehat{S}_j^\alpha \right) \right]^2 \right\}. \tag{4}$$

The HS fields can be evaluated self-consistently to be $\Delta_{ij} = \gamma_1 \Delta_{ij}^0$, $\chi_{ij} = \gamma_2 \chi_{ij}^0$ and $S_{ij}^\alpha = \gamma_3 S_{ij}^{\alpha,0}$. By employing the single occupancy constraint, we rewrite and decompose the term in Eq. (3) by using the HS transformation and obtain $\widehat{n}_i \widehat{n}_j = (1/2) [(\widehat{n}_i + \widehat{n}_j)^2 - (\widehat{n}_i^2 + \widehat{n}_j^2)] \rightarrow (1/2)(3 - 4\delta)(\widehat{n}_i + \widehat{n}_j) - 2(1 - \delta)^2$. The factor $2\gamma_2^2 + \gamma_3^2$ contained in the fifth term of Eq. (3) must be carefully treated when the HS transformation is applied. Noting that for the requirement of normalization of HS transformation:

$$\sqrt{\alpha/\pi} \int_{-\infty}^{\infty} dx \exp \left[-\alpha (x - \widehat{x})^2 \right] = 1,$$

the prefactor $\sqrt{\alpha/\pi} = \exp \left(\frac{1}{2} \ln \frac{\alpha}{\pi} \right)$ must be included as decoupling some operator \widehat{x}^2 ; and this factor could be absorbed into the mean-field Hamiltonian as an extra term: $-\frac{1}{2} \ln \alpha$. If α is a constant, then its presence will not introduce any effect. However, α is *not* a constant in our decoupling of the $\widehat{n}_i \widehat{n}_j$ term, instead it is $2\gamma_2^2 + \gamma_3^2$, which is a variable. Therefore, it will introduce some important effects in the mean-field Hamiltonian when we minimize the free energy with respect to γ_i . The t term in Eq. (3) can be decomposed as $\widehat{\chi}_{ij} \widehat{G}_{ji} \rightarrow \chi_{ij}^0 \widehat{G}_{ji} + G_{ji}^0 \widehat{\chi}_{ij} - \chi_{ij}^0 G_{ji}^0$ by introducing two decoupling fields χ_{ij}^0 , G_{ji}^0 . According to Ref. [8], the spin singlet order parameter is assumed as: $\Delta_{ij} = \Delta e^{\pm i\tau}$, where the plus sign refers to $j = i \pm \widehat{x}$ and otherwise; the order parameter χ_{ij} (χ_{ij}^0 , G_{ji}^0) is assumed to be staggered: $\chi_{ij} = \chi e^{\pm i\varphi}$ ($\chi_{ij}^0 = \chi^0 e^{\pm i\varphi}$, $G_{ji}^0 = G^0 e^{\pm i\varphi}$), where the plus sign is taken as the direction $j \rightarrow i$ is the same as that indicated in Fig. 1 and minus sign is taken otherwise. Note that χ_{ij}^0 and G_{ji}^0 , instead of G_{ij}^0 , are assumed to be in phase. The Néel order is assumed to be along the z -direction only: $S_{ij}^z = (-)^i S = (-)^i \gamma_3 S^0$, $S_{ij}^x = S_{ij}^y = 0$, where $(-)^i = +1$ if position i belongs to the A sublattice and $(-)^i = -1$ otherwise. This is equivalent to the case that sublattice A is dominated by spin-up spinons and sublattice B by spin-down spinons. It is noted that there is no local $SU(2)$ symmetry even at half filling, when $S \neq 0$ and the spin singlet order parameter no longer has to be the d -wave. (Strictly speaking, if γ are not set to be

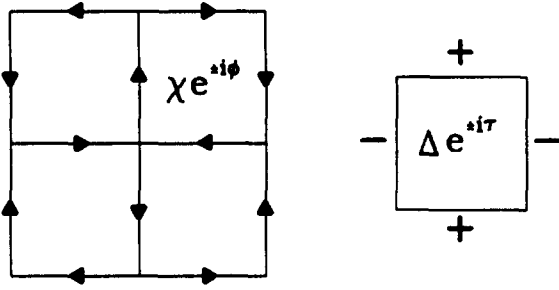


Fig. 1. Each vertex in the above figures corresponds to a lattice site. The phase of $\chi_{ij} = \chi e^{\pm i\phi}$ is $+\phi$ if the direction $j \rightarrow i$ points along the arrow on the bond and is $-\phi$ otherwise. As a result, χ_{ij} has a staggered flux of 4ϕ on each plaquette. $\Delta_{ij} = \Delta e^{\pm i\tau}$ is given a phase $+\tau$ ($-\tau$) if the bond ij is in the \hat{x} (\hat{y}) direction.

constant, local $SU(2)$ symmetry does not exist even when $S = 0$.)

With the above assumptions, the mean-field Hamiltonian can be written as ($J = 1$):

$$H_{MF} = \sum_k \boldsymbol{\eta}^+ M_k \boldsymbol{\eta} + \sum_k \boldsymbol{\zeta}^+ N_k \boldsymbol{\zeta} + R, \quad (5)$$

where

$$\boldsymbol{\eta}^+ = \begin{bmatrix} f_{k\uparrow}^{A+} & f_{k\downarrow}^{B+} & f_{-k\downarrow}^A & f_{-k\uparrow}^B \end{bmatrix},$$

$$\boldsymbol{\zeta}^+ = \begin{bmatrix} b_k^{A+} & b_k^{B+} \end{bmatrix},$$

$$M_k = \begin{bmatrix} -\mu_\uparrow & \varepsilon_k & 0 & \Delta_k \\ \varepsilon_k^* & -\mu_\downarrow & \Delta_{-k} & 0 \\ 0 & \Delta_{-k}^* & \mu_\downarrow & -\varepsilon_k^* \\ \Delta_k^* & 0 & -\varepsilon_k & \mu_\uparrow \end{bmatrix}, \quad (6)$$

$$N_k = \begin{bmatrix} -\mu_b & \varepsilon_k^b \\ \varepsilon_k^{b*} & -\mu_b \end{bmatrix},$$

$$R = \frac{N}{2} \left[2(\Delta^2 + \chi^2 + S^2 + \mu_b - \bar{\mu}) + 8tG_0\chi_0 + (2\gamma_2^2 + \gamma_3^2)(1 - \delta)^2 \right] - \frac{1}{2} \ln(2\gamma_2^2 + \gamma_3^2).$$

In the above expression, we have redefined the spin-up (-down) spinon to be spin-down (-up) on sublattice B and the summation over k is restricted to the reduced Brillouin zone. The Hamiltonian is similar to that of Ref. [19], which employed the renormalized mean-field approach. In the above expression, N is the number of sites, $\varepsilon_k = -\gamma_2(\chi + 2tG^0/\gamma_2)\gamma_k^\varphi$, $\varepsilon_k^b = -2t\chi^0\gamma_k^\varphi$, $\gamma_k^\varphi = e^{i\varphi} \cos k_x a + e^{-i\varphi} \cos k_y a$, $\Delta_k = \gamma_1 \Delta \gamma_k^i$, and $\mu_b = ia_0$ is the mean value of the Lagrangian multiplier and can be treated as the chemical

potential of holon, $\bar{\mu} = \mu + \mu_b - \gamma_2^2 - (3/2)\gamma_3^2 + (1 - \delta)(2\gamma_2^2 + \gamma_3^2)$, $\mu_\uparrow = \bar{\mu} + 2\gamma_3 S$, and $\mu_\downarrow = \bar{\mu} - 2\gamma_3 S$. The last two expressions play the roles of chemical potentials of the (redefined) spin-up and spin-down spinon, respectively.

We would like to emphasize some important effect here. The γ_1 -term contributes to the mean-field Hamiltonian as a form like: $\Delta_k f_{k\uparrow}^{A+} f_{-k\downarrow}^{B+} + \text{h.c.}$ and the γ_2 term contributes as the form like: $-\gamma_2 \chi \gamma_k^\varphi f_{k\uparrow}^{A+} f_{k\downarrow}^B + \text{h.c.}$ Since $\Delta_k \propto \gamma_k^r$, which is non-zero in the entire Brillouin zone rather than in the vicinity of Fermi surface only as the conventional s -wave superconductor does, the γ_1 term contributes to the dynamics of the system in the entire Brillouin zone instead of in the neighborhood of Fermi surface. Furthermore, the γ_2 term contributes to the dynamics mainly in the region of the momentum space below the Fermi energy. As a result, the regions of momentum space, where these two terms contribute significantly to the system, overlap with each other. Therefore, in the Hartree-Fock approach, the assumption of $\gamma_1^2 = \gamma_2^2 = \gamma_3^2 = 1$ would result in overcounting of the dynamics displayed by the exchange term and the path integral method which requires $\gamma_1^2 + \gamma_2^2 + \gamma_3^2 = 1$ should be more reliable.

As a usual procedure, the Hamiltonian in Eq. (5) can be diagonalized by unitary transformation. Therefore, the free energy can be written as

$$F = -\frac{1}{\beta} \sum_{k, \sigma = \pm, n} \left[\ln(1 + e^{-\beta E_{nk}^f}) - \ln(1 - e^{-\beta E_{k\sigma}^h}) \right] + R, \quad (7)$$

where

$$E_{2k}^f = -E_{1k}^f, \quad E_{4k}^f = -E_{3k}^f,$$

$$E_{mk}^f = \left[2(\bar{\mu}^2 + |\varepsilon_k^\varphi|^2) + 2|\Delta_k|^2 + 8\gamma_3 S \left(\gamma_3 S \pm \sqrt{\bar{\mu}^2 + |\varepsilon_k^\varphi|^2} \right) \right]^{1/2},$$

with a plus (minus) sign for $m = 1(3)$ and $E_{k\pm}^h = \pm |\varepsilon_k^b| - \mu_b$. The saddle point solution can be obtained by minimizing the free energy with respect to auxiliary fields Δ , χ , S , G^0 , φ , τ , $\bar{\mu}$ and μ_b . These yield the following nine simultaneous equations:

$$\begin{aligned}
0 &= \left[-\gamma_1^2 \sum_k^{n=1,3} \frac{|\gamma_k^f|^2}{E_{nk}^f} \tanh \left(\frac{\beta E_{nk}^f}{2} \right) + N \right] \Delta, \\
0 &= -\gamma_2^2 \xi \left\{ \sum_k^{n=1,3} \frac{|\gamma_k^\varphi|^2}{E_{nk}^f} \left(1 \pm \frac{2\gamma_3 S}{\sqrt{\mu^2 + |\varepsilon_k^\varphi|^2}} \right) \right. \\
&\quad \left. \times \tanh \frac{\beta E_{nk}^f}{2} \right\} + N\chi, \\
0 &= -2\gamma_3 \left\{ \sum_k^{n=1,3} \frac{1}{E_{nk}^f} \left(2\gamma_3 S \pm \sqrt{\mu^2 + |\varepsilon_k^\varphi|^2} \right) \right. \\
&\quad \left. \times \tanh \frac{\beta E_{nk}^f}{2} \right\} + NS, \\
\chi &= \gamma_2 \chi^0, \\
0 &= \sum_k [f^h(E_{k+}^h) - f^h(E_{k-}^h)] |\gamma_k^\varphi| + 2NG^0, \\
0 &= \sin(2\varphi) \left\{ - \sum_k^{n=1,3} \gamma_2^2 \xi^2 \frac{\cos k_x a \cos k_y a}{E_{nk}^f} \right. \\
&\quad \times \left(1 \pm \frac{2\gamma_3 S}{\sqrt{\mu^2 + |\varepsilon_k^\varphi|^2}} \right) \tanh \frac{\beta E_{nk}^f}{2} \\
&\quad \left. + \sum_k [f^h(E_{k+}^h) - f^h(E_{k-}^h)] 2t\chi^0 \right. \\
&\quad \left. \times \frac{\cos k_x a \cos k_y a}{|\gamma_k^\varphi|} \right\}, \\
0 &= \sin(2\tau) \sum_k^{n=1,3} \gamma_1^2 \Delta^2 \frac{\cos k_x a \cos k_y a}{E_{nk}^f} \tanh \frac{\beta E_{nk}^f}{2}, \\
N\delta &= - \sum_k^{n=1,3} \frac{2\bar{\mu}}{E_{nk}^f} \left(1 \pm \frac{2\gamma_3 S}{\sqrt{\mu^2 + |\varepsilon_k^\varphi|^2}} \right) \tanh \frac{\beta E_{nk}^f}{2}, \\
N\delta &= \sum_k [f^h(E_{k+}^h) + f^h(E_{k-}^h)],
\end{aligned} \tag{8}$$

where the \pm sign is used to represent that plus sign is taken for $n = 1$ and minus sign is taken for $n = 3$. If we take γ_1 and γ_2 as free parameters and minimize F with respect to them, then by using the above simultaneous equations we obtain the following two simple relations between the order parameters:

$$(\chi^0)^2 - (\Delta^0)^2 = 2\delta(1 - \delta), \tag{9}$$

$$(S^0)^2 - (\chi^0)^2 = (1 - \delta)^2 - \frac{1}{1 - \gamma_1^2 + \gamma_2^2}. \tag{10}$$

The second term on the right-hand side of Eq. (10) is important in determining the order parameters of the system. It comes from the careful treatment of the normalization constant introduced by the HS transformation on the $\hat{n}_i \hat{n}_j$ term as mentioned above. An important conclusion can be made from Eqs. (9) and (10) that because of the minus sign between order parameters contained in the above two equations, it manifests that these three order parameters favor coexistence rather than competition with each other.

Fig. 2 presents the result of the saddle point solution. It shows the variation of three order parameters with temperature for $\delta = 0$ and 0.05 . All the results presented in this work correspond to the d -wave ($\tau = \pi/2$) except those shown in Fig. 4, where the $s + id$ -wave, π flux state is also presented. In contrast with previous works, the π -flux ($\varphi = \pi/4$) can not be obtained in our work as the RVB order is the d -wave, instead, the staggered flux ($= 4\varphi$) changes from 0 to about 1.4 as the doping increases from 0 to critical doping. Previous work showed the d -wave together with the π -flux phase is the lowest energy solution when $\delta = 0$. This state is equivalent to the pure RVB $s + id$ -wave state by a local $SU(2)$ transformation. The absence of this solution in our works

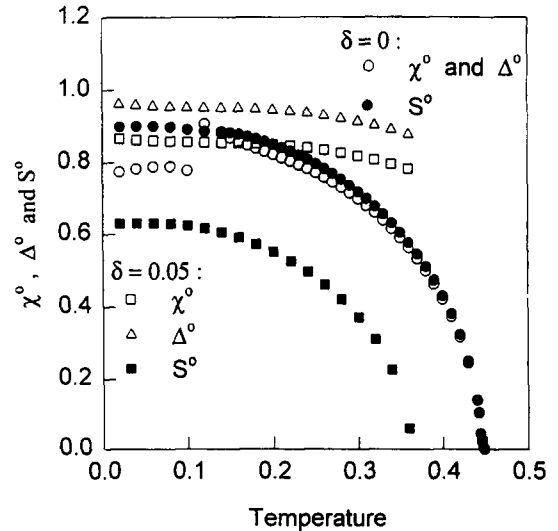


Fig. 2. The variation of χ^0 , Δ^0 and S^0 with temperature for the d -wave ($\tau = \pi/2$) solution. The doping $\delta = 0.0$ and $\delta = 0.05$ are shown here.

may be due to the absence of local $SU(2)$ symmetry when the Néel order is introduced. At half filling, it shows that $\chi^0 = \Delta^0$, as can be seen from Eq. (9). Our result shows that all of the three order parameters fall to zero when $\delta = 0$ as temperature exceeds the Néel temperature, T_N . This implies that, at exact half filling, the phase changes from antiferromagnetic state to paramagnetic state when T is larger than T_N , which is consistent with experiments.

The values of γ for d -wave and $s+id$ -wave solutions are found to be almost constant for temperatures from 0 to T_N . They are approximately $\gamma_1 \sim 0.7$, $\gamma_2 \sim 0.5$ and $\gamma_3 \sim 0.45$ when $\delta = 0.05$, and $\gamma_1 \sim 0.6$, $\gamma_2 \sim 0.66$, $\gamma_3 \sim 0.35$ when $\delta = 0$ respectively. With $J \sim 0.1$ eV, $\delta = 0$ one obtains the Néel temperature $T_N \simeq 0.45J \sim 530$ K, which is about twice the value of that of La_2CuO_4 . Inaba et al. [15] used the standard Hartree-Fock decoupling scheme and took the spin density wave mean field on the spin-spin interaction sector. Their result yielded a value of $T_N = 0.5J$ for $t/J = 4$. One can note that our result agrees quite satisfactorily with their result.

Fig. 3 shows how doping affects the order parameters at a constant temperature $T = 0.1J$. When $\delta = 0$, the exact value of staggered magnetization $m (= |\langle \hat{S}_{i,z} \rangle|)$ is yet unknown and various numerical simulations have been performed by variational and Monte Carlo methods. The calculated results of m range from

0.42 to 0.3 [20]. In our work, the staggered magnetization m was calculated from the parameter $S^0 \sim 0.92$. The value of m was shown to be $m = 0.46$, which is slightly larger than the upper bound of the previous numerical results [20]. Inaba et al. [15] also calculated the staggered magnetization, however, their results cannot provide a reasonable m . In their work, the calculated result of $m \simeq 1$ exceeded the saturation value ($m \leq 0.5$). Therefore, our decoupling scheme is more reasonable and better than that of Ref. [15]. Our work also shows that staggered magnetization drops quickly as holes are introduced. The other two order parameters are less affected by holes and do not approach zero when the Néel temperature is attained.

Fig. 4 presents the phase diagram for the d -wave and $s + id$ -wave in t - J model. There is a cusp near $\delta = 0.01$ for both cases. The cusp may be introduced artifactly by our approximation on the holon part. In evaluating our results, we have frozen the holon part, i.e. we assume all the states are Bose condensed to the lowest energy state for any temperature and hole concentration. This is a good numerical approximation except for holons being far away from condensation. This occurred for small δ and high temperature, and it just happens in the case of the cusp. Although, our calculated critical doping is $\delta_c = 0.068(0.9)$ for the d -wave ($s + id$ -wave) which is three (four) fold larger than that of La_2CuO_4 , however, our results are still

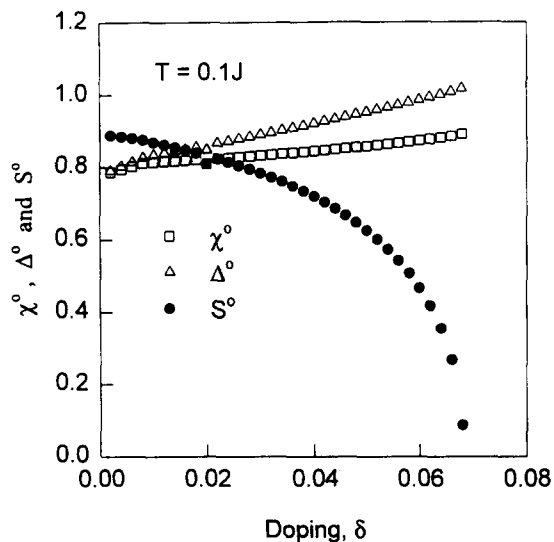


Fig. 3. The variation of χ^0 , Δ^0 and S^0 with doping, δ for the d -wave solution. The temperature is fixed at $0.1J$.

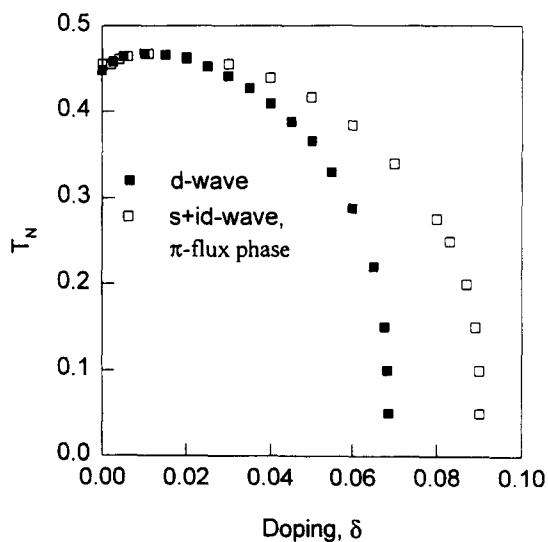


Fig. 4. Phase diagrams for the d -wave and $s + id$ -wave (π -flux phase), respectively.

smaller than that obtained by Ref. [15] which gave a value of $\delta_c \simeq 0.15$.

The region below T_N is the antiferromagnetic phase where $S^0 \neq 0$. The region above T_N , where $S^0 = 0$, and/or beyond critical doping can be divided into two regions according to whether Bose–Einstein condensation occurred or not. The region is superconducting if it is below the Bose–Einstein condensation temperature and is a pseudospin state otherwise. It is still an open question whether spin singlet order leads to superconducting when the Néel order exists. The interplay between these two orders is interesting and deserves future study.

In conclusion, we have shown the coexistence of the Néel order, the flux phase and the RVB state. Simple relations are obtained among order parameters by optimizing the free energy with respect to the various γ . The connection between the antiferromagnetic state and the superconducting state can be obtained when the hole concentration is varied.

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