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1. Introduction

The two-dimensional layers of cuprate oxides are known to be the systems of strongly repulsive (correlated) electrons as the Mott insulators which have revealed various novel physical properties uniquely different from the conventional low temperature superconductors. They show the antiferromagnetic (AF) infinite-range or long-range order (AFLRO) at and near half-filling. As hole doping increases, the AFLRO diminishes and the short-range (finite-range) AF order takes over with the emergence of d-wave superconductivity. The two-dimensional systems of strongly correlated electrons involved with strong repulsive interactions may favor the spin singlet pairing order (or correlations) of d-wave symmetry over that of s-wave symmetry. Here the spin singlet paring correlations are concerned with the AF spin fluctuations of the shortest possible correlation length among the AF spin fluctuations of all possible correlation lengths which appear in the region of hole doping away from half-filling. In this region of hole doping the cuprate oxides exhibit the novel structure of the high $T_C$ phase diagram characterized by the dome-shaped superconducting transition temperature, $T_C$, and the monotonously decreasing pseudogap temperature, $T^\ast$.

Earlier, slave-boson approaches of the t-J Hamiltonian were proposed by researchers in the field[1–3] in an attempt to reproduce the observed high $T_C$ phase diagram. They were successful in reproducing the monotonously decreasing pseudogap temperature $T^\ast$ in agreement with observation. $T^\ast$ is shown to be the spin gap temperature at which the spin singlet pairing order or the spin (spinon) pairing correlations begins to open. However, their treatment of single-holon bose condensation has led to a linear increase of the bose condensation temperature $T_C$ rather than the observed dome-shaped $T_C[2, 3]$. Later we introduced a slave-boson approach which allows the double-holon bose condensation[4] and failed to reproduce the dome-shaped $T_C$, also yielding the linearly increasing trend of $T_C$. 

Role of Antiferromagnetic Fluctuations in High Temperature Superconductivity

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Soon after this study we[5] proposed an improved slave-boson theory which fundamentally differs from these approaches in that a term involving coupling between the spin and charge degrees of freedom or simply spin-charge coupling appears in our rigorous slave-boson treatment of the t-J Hamiltonian. The resulting effective mean field Lagrangian reveals coupling between the spin (spinon) paring order, $\Delta^f$, and the charge (holon) paring order, $\Delta^b$. As a consequence the Cooper pairing order is satisfactorily seen to be a composite of these two order parameters, $\Delta^f$ and $\Delta^b$ to allow for the boson condensation of the Cooper pairs rather than the single-holon boson condensation or the double-holon boson condensation. Accordingly this theory has led to successful reproductions of not only the monotonously decreasing spin gap temperature but also the long-waited dome-shaped structure of the superconducting transition temperature in the phase diagram. Further other important physical observations such as the boomerang behavior of superfluid weight, the peak-dip-hump structure of optical conductivity and both the temperature and doping dependence of spectral functions are reproduced in agreement with observations[6].

For the sake of self-containment we will first review our earlier proposed slave-boson theory[5] of the t-J Hamiltonian which reveals the spin-charge coupling mentioned above. Earlier it was shown by others that inclusion of the $t'$ term in the t-J Hamiltonian leads to satisfactory descriptions of the electronic structure of high $T_C$ cuprates[7–11] and the enhancement of pairing correlation resulting in an increasing trend of $T_C$ in the overdoped region in the phase diagram for the choice of $t'/t < 0$, e.g., $t'/t = -0.3[12, 13]$. It is, thus, of great interest to see how its inclusion affects the entire structure of the phase diagram which includes the pseudogap temperature. At present there has been no study which addresses the role of the diagonal hopping $t'$ on the spin gap temperature, $T^*$. Such study is needed to find whether there exists any relation between $T^*$ and $T_C$ or the spin gap phase and the superconducting phase. In this regard we would like to draw attention to the fact that the observed phase diagrams of high $T_C$ cuprate samples (e.g., LSCO and BSCCO samples) reveal that higher the $T^*$, higher the $T_C$ as earlier discussed by Oda et al.[14]. This suggests that the two energy or temperature scales, $T^*$ and $T_C$ are no longer independent of each other. Thus one of our main objectives is to study how the pseudogap or spin gap temperature, $T^*$ and the superconducting transition temperature, $T_C$ are correlated and show that such correlation arises owing to the presence of the short-range antiferromagnetic (AF) spin fluctuations of the shortest possible correlation length involved with the spin pairing correlations. For a concerted, self-consistent study, we use a predicted phase diagram to calculate magnetic susceptibility and discuss two important observations made by the inelastic neutron scattering (INS) measurements, namely the temperature dependence of the magnetic resonance peak[17] and the linear scaling behavior between the magnetic peak resonance energy, $E_{res}$, and the superconducting transition temperature[18]. From this study we show that the short-range AF spin fluctuations are directly responsible for the magnetic susceptibility observed by the INS measurements mentioned here.

2. Theory: U(1) slave boson representation of the t-J Hamiltonian

In the present study we limit ourselves to the derivation of the U(1) slave boson representation of the t-J Hamiltonian. We refer details of its derivation to Appendix A. In Appendix B a brief exposure of the SU(2) approach is made in association with the U(1) representation. Here only a rudimentary description is presented by introducing the next-nearest neighbor hopping or
diagonal hopping \( t' \) term into the \( t - J \) Hamiltonian. It is given by,

\[
H_{t-t'-J} = -t \sum_{<ij>} (c_i^\dagger \epsilon_{ij} c_j + c.c.) - t' \sum_{<ij>',} (\tilde{c}_i^\dagger \epsilon_{ij} \tilde{c}_j + c.c.) + J \sum_{<ij>} (S_i \cdot S_j - \frac{1}{4} n_i n_j).
\]

(1)

Here \( \sum_{<ij>} \) denotes summation over the nearest neighbor sites \( i \) and \( j \), \( \sum_{<ij>,} \) the summation over the next-nearest neighbor (diagonal) sites and \( \tilde{c}_{ij}(\epsilon_{ij}^\dagger) \), the electron annihilation(creation) operator with the constraint of no double occupancy at each site \( i \). \( t \) is the nearest neighbor hopping integral; \( t' \), the next-nearest neighbor hopping integral and \( J \), the Heisenberg coupling constant.

We take the slave-boson representation of electron operator as a composite of spinon (\( \lambda \)) and holon (\( b \)), that is, \( c_{i\sigma} = f_{i\sigma} b_i^\dagger \) with the single occupancy constraint at each site \( i \). Following a rigorous slave-boson treatment of \( S_i = \frac{1}{2} \sum_{\alpha, \beta} \epsilon_{i\alpha}^\dagger \epsilon_{i\beta} \sigma_{\alpha\beta} \) with \( \sigma_{\alpha\beta} \) the Pauli spin matrix

in the above equation, the resulting U(1) slave-boson representation of the above \( t - t' - J \) Hamiltonian is given by

\[
H_{t-t'-J} = -t \sum_{<ij>,\sigma} (f_{i\sigma}^\dagger f_{j\sigma} b_i^\dagger b_j + c.c.) - t' \sum_{<ij>',\sigma} (f_{i\sigma}^\dagger f_{j\sigma} b_i^\dagger + c.c.)
- \frac{1}{2} \sum_{<ij>} b_i b_j b_i^\dagger b_j^\dagger (f_{i\uparrow}^\dagger f_{j\uparrow}^\dagger - f_{i\downarrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow} - f_{i\uparrow}^\dagger f_{j\downarrow})
+ t \sum_i \lambda_i (\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1).
\]

(2)

Here \( \lambda_i \) is the Lagrange multiplier field which enforces the single occupancy constraint.

Taking proper Hubbard-Stratonovich transformations and associated algebras by closely following our recently proposed slave-boson theory[5] (see Appendix A for details), one obtains the following effective Lagrangian,

\[
\mathcal{L}_{\text{eff}} = \mathcal{L}_0 + \mathcal{L}_f + \mathcal{L}_b
\]

(3)

with

\[
\mathcal{L}_0 = \frac{J}{2} \sum_{<ij>,\sigma} \left| \Delta_{ij} \right|^2 + \frac{1}{2} \left| \chi_{ij} \right|^2 + \frac{1}{4} \right) + \frac{J}{2} \sum_{<ij>,\sigma} \left| \Delta_{ij} \right|^2 (\left| \Delta_{ij} \right|^2 + \chi^2),
\]

(4)

\[
\mathcal{L}_f = \sum_{\sigma} f_{i\sigma}^\dagger (\partial \tau - p^\dagger) f_{i\sigma}
- \frac{J}{4} \sum_{<ij>,\sigma} \left\{ \chi_{ij}^\dagger f_{i\sigma}^\dagger f_{j\sigma} + c.c. \right\}
- t' x \sum_{<ij>,\sigma} \left\{ f_{i\sigma}^\dagger f_{j\sigma} + c.c. \right\}
- \frac{J}{2} \sum_{<ij>,\sigma} \left\{ \Delta_{ij}^\dagger (f_{i\downarrow}^\dagger f_{j\downarrow} - f_{i\uparrow}^\dagger f_{j\uparrow}) + c.c. \right\},
\]

(5)
for the spin spinon sector and
\[
\mathcal{L}_b = \sum_i b_i^\dagger (\partial_\tau - \mu b) b_i - t \sum_{\langle i,j \rangle} \left\{ \chi_{ij} b_i^\dagger b_j + c.c. \right\} \\
- t'(1-x) \sum_{\langle i,j \rangle} \left\{ b_i^\dagger b_j + c.c. \right\} \\
- \frac{J}{2} \sum_{\langle i,j \rangle} |\Delta_{ij}^f|^2 \left\{ \Delta_{ij}^b b_i^\dagger b_j + c.c. \right\},
\]
(6)
for the charge (holon) sector. Here \( \mu^f (\mu^b) \) is the spinon(holon) chemical potential. \( \chi_{ij} \) is the hopping order parameter and \( \Delta_{ij}^f = < f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} > \), \( \Delta_{ij}^b = < b_i b_j > \), the spinon (holon) pairing order parameter; \( x \), the hole doping concentration and \( f_x = j(1-x)^2 \). The last term of Eq. 6 reveals the presence of coupling between the spin (spinon) and charge (holon) degrees of freedom, i.e., simply termed as spin-charge coupling, as seen in the form of the product of the spin (spinon) single pairing order, \( \Delta^f \) and the charge (holon) pairing order, \( \Delta^b \). Thanks to this coupling the Cooper pairing order \( \Delta \) is, now, properly represented as a composite of these two order parameters, \( \Delta^f \) and \( \Delta^b \). We point out that the holon (charge) sector, Eq. 6 is coupled with the spinon (spin) sector, Eq. 5 owing to the presence of coupling between the spinon pairing order \( \Delta^f \) and the holon pairing order \( \Delta^b \) as shown in the last term of Eq. 6.

The resulting free energy (see derivation in Appendix A) is given by,
\[
F = - \frac{1}{\beta} \ln Z \\
= JzN \left( 2|\Delta^f|^2 + \frac{1}{2} |\chi|^2 \right) + JN|\Delta^f|^2 |\Delta^b|^2 \\
-(1-x)N\mu_{\text{eff}}^f + Nx\mu_{\text{eff}}^b + \frac{1}{2} \sum_k E_k^{\text{bs}} \\
-2Nk_B T \ln 2 - 2k_B T \sum_k \cosh \frac{\beta E_k^{\text{bs}}}{2} \\
+ k_B T \sum_k \ln \left( 1 - e^{-\beta E_k^{\text{bs}}} \right),
\]
(7)
where \( Z = \int \mathcal{D}f \mathcal{D}b \mathcal{D}\chi \mathcal{D}\Delta^f \mathcal{D}\Delta^b \mathcal{D}\lambda e^{-\int_0^\beta d\tau \mathcal{L}_{\text{eff}}} \) is the partition function; \( \Delta^f = < f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} > \), \( \Delta^b = < b_i b_j > \), the spinon(holon) pairing order parameter; \( E_k^f = \sqrt{(\epsilon_k^f - \mu_{\text{eff}}^f)^2 + \Delta^f_k^2} \) and \( E_k^b = \sqrt{(\epsilon_k^b - \mu_{\text{eff}}^b)^2 + \Delta^b_k^2} \), the spinon(holon) quasiparticle energy; \( x \), the hole doping rate; \( f_x = j(1-x)^2 \) and \( N \), the total number of sites in a square lattice. Here the spinon and holon energies, \( \epsilon_k^f \) and \( \epsilon_k^b \) are respectively,
\[
\epsilon_k^f = - \frac{J}{2} \chi (\cos k_x + \cos k_y) - 4t'x \cos k_x \cos k_y \\
\epsilon_k^b = -2t \chi (\cos k_x + \cos k_y) - 4t'x \cos k_x \cos k_y.
\]
(8)
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The contribution of the next-nearest neighbor hopping or the diagonal hopping is readily understood from the inspection of Eq.8 by noting that the value of \( \cos k_x \cos k_y \) is negative at the hot spot \((\pi, 0)\), zero at the cold spot \((\pi/2, \pi/2)\) and positive at \((0, 0)\). From this we see that stabilization (destabilization) of the spinon energy at the hot spot with \( t' < 0 \) \(( t' > 0 \) is expected to lead to the enhancement (depression) of AF spin (spinon) pairing correlations or the spin singlet pairing order of d-wave symmetry compared to the case of \( t' = 0 \), that is, no diagonal hoping. The charge (holon) pairing of s-wave symmetry will be enhanced at the nodal points.

3. Role of next-nearest neighbor hopping on the structure of phase diagram

Here we explore the role of the next-nearest neighbor hopping, i.e., the diagonal hopping on both the pseudogap temperature \( T^* \) and the superconducting transition temperature, \( T_C \) and the cause of correlation between these two temperature scales or relatedly the spin gap phase and the d-wave superconducting phase. Earlier the negative value of \( t' \) was shown to match well the observed Fermi surface of the hole doped cuprate oxides while its positive value matches that of the electron doped cuprate oxides[7] as mentioned above.

Choosing the two different cases of the diagonal hopping, one for \( t' < 0 \) \(( e.g., t' = -0.3t)\) and the other for \( t' > 0 \) \(( e.g., t' = 0.3t)\), we examine the dependence of the phase diagram on \( t' \) for the hole doped cuprate oxides.

Fig.1 shows the computed results of the phase diagram with the variation of \( t'/t \) at a fixed value of the Heisenberg coupling constant, \( J = 0.3t \). In the underdoped region both \( T^* \) and \( T_C \) are predicted to remain largely unchanged despite the considerable change of \( t'/t \).
from a positive value \( t' / t = 0.3 \) to a negative \( t' / t = -0.3 \) one. On the other hand, in the overdoped region both \( T^* \) and \( T_C \) are seen to simultaneously increase (decrease) for the case of \( t' / t < 0 \) (\( t' / t > 0 \)) with reference to that of \( t' / t = 0 \). The predicted superconducting transition temperature at optimal doping concentration did not change appreciably despite the considerable variation of \( t' / t \) as shown in the figure. The simultaneous increase (decrease) of \( T^* \) and \( T_C \) with \( t' / t = -0.3 \) (\( t' / t = 0.3 \)) indicates that the two temperature scales, \( T^* \) and \( T_C \) or the spin gap phase and the superconducting phase are interrelated. To see the cause of such interplay, below we probe the role of the short-range AF spin fluctuations or the spin pairing correlations on the determination of the phase diagram.

For the case of \( t' < 0 \) (\( t' > 0 \)) the spinon energy at the hot spot\((\pi,0)\) is lowered (raised) with reference that of \( t' = 0 \), i.e., no diagonal hopping, as can be readily understood from Eq. 8. Thus the spin (spinon) pairing correlation at the hot spot for \( t' < 0 \) is energetically more stable than the case for \( t' > 0 \). It is to be recalled that the spin gap temperature is the temperature at which the spin singlet paring order or (correlations) of d-wave symmetry or the spin pairing correlations emerges. The spin pairing correlations will be less prone to change in the underdoped region compared to the case of the overdoped region. This is because owing to lower hole concentrations in this region, chances of electron hopping from site to site are reduced and, consequently, the existing short-range AF order is not easily perturbed. Thus the spin pairing correlations or the short-range antiferromagnetic spin fluctuations is expected to remain more robust in the underdoped region compared to the case of the overdoped region. Indeed, the predicted \( T^* \) and \( T_C \) is shown to be sensitive to the variation of \( t' \), preferentially in the overdoped region. This is displayed in Fig. 1.

It is reminded that the Cooper pairing order can be seen as the composite of the spin (spinon) pairing order \( \Delta^s \) and the charge (holon) pairing order \( \Delta^b \), which results from the presence of the spin-charge coupling shown in the last term of Eq. 6. As a result of the coupling between the two orders, the superconducting phase transition with its onset temperature, \( T_C \) may arise owing the short-range AF spin fluctuations involved with the formation of the spin pairing order (correlations) which initiates the onset of the spin gap temperature \( T^* \). To put it otherwise, owing to the spin-charge coupling both \( T^* \) and \( T_C \) are simultaneously affected or correlated. Indeed, such simultaneous change is seen to appear by exhibiting the simultaneous increase (decrease) of both \( T^* \) and \( T_C \) with \( t' / t < 0 \) (\( t' / t > 0 \)) as \( J \) increases. Such trend is seen in Fig. 2. Our findings of both the enhancement of the spin pairing correlations and the increasing trend of the superconducting transition temperature for \( t' = -0.3t \) which appear in the overdoped region agree well with the variational Monte Carlo, mean-field calculations of Lee and coworkers [13]. However, unlike our present study they did not show a study of the spin gap temperature concerned with the role of the spin pairing correlations.

For further verification from a different angle we closely examine the predicted structural dependence of the phase diagram on \( J \) in Fig. 2. Both \( T^* \) and \( T_C \) are predicted to simultaneously increase with \( J \) as shown in Fig. 2. Needless to say, spin pairing correlations should increase with \( J \). This will, in turn, cause the simultaneous increase of both the spin gap temperature and the superconducting transition temperature with increasing \( J \). Such simultaneous increase with \( J \) is predicted as shown in the figure. This clearly demonstrates that the the superconducting transition temperature and the pseudogap temperature or relatedly the spin gap phase and the d-wave superconducting phase are correlated via the spin pairing correlations or the AF spin fluctuations of the shortest possible correlation length.
To put it otherwise, the short-range AF spin fluctuations play a key role of causing such inseparable relation between the two temperature scales or relatedly the spin gap phase and the superconducting phase. This finding is consistent with the observed phase diagrams with different cuprate samples which shows higher the $T^*$, higher the $T_C$[14] as mentioned earlier. It is then assured that the superconducting phase transition will not arise in the absence of the spin gap phase below $T^*$ which is initiated by the short-range AF spin fluctuations involved with the spin paring correlations.

4. Magnetic susceptibility based on the U(1) slave-boson representation

The observed high $T_c$ phase diagrams of cuprate oxides are characterized by the pseudogap or spin gap phase which exists below the monotonously decreasing $T^*$ and the d-wave superconducting phase below the dome shaped $T_C$[15, 16]. From their inelastic neutron scattering measurements (INS) of the temperature dependence of magnetic resonance peaks for YB$_2$Cu$_3$O$_{6+x}$ (YBCO) Dai et al. [17] reported that the magnetic resonance begins to appear at the pseudogap temperature $T^*$ as its onset temperature and continues to exist with an increasing trend of the resonance peak height in the underdoped region as temperature is lowered and that near the optimal doping $T^*$ tends to get closer to $T_c$. On the other hand, He et al. observed from their INS measurements of the doping dependence of the resonance peak energy, $E_{res}$ for Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO) that in the underdoped region $E_{res}$ increases with increasing hole concentration $x$ up to optimal doping $x_0$, and that in the overdoped cuprates it decreases with increasing $x$, by exhibiting a linear scaling behavior of $E_{res}$ with $T_c$ at all hole concentrations[18]. Most recently Stock et al.[19] observed that spin waves decay above the pseudogap of a heavily underdoped YBCO. Using a time-of-flight neutron spectroscopy for the studies of dynamic spin correlations or spin fluctuations in the overdoped La$_{2-x}$Sr$_x$CuO$_4$
(LSCO) sample, Wakimoto et al.[20] showed from their study of the doping dependence of antiferromagnetic spin excitations that the excitations decrease with hole doping above the optimal doping of $La_{2-x}Sr_xCuO_4$ (LSCO) and disappear at $x = 0.3$. Here we discuss the magnetic susceptibility[21, 22] at the wave vector $\vec{Q} = (\pi, \pi)$ in association with our computed phase diagram and focus our attention to the observed linear scaling behavior of magnetic resonance peak energy $E_{\text{res}}$ with the superconducting transition temperature $T_c$. For self-containment we first discuss the U(1) slave-boson representation of irreducible magnetic susceptibility for our calculations of magnetic susceptibility.

Allowing external magnetic field $\vec{h}$, we introduce into the effective Lagrangian $L_{\text{eff}}$ above the Zeeman coupling term,

$$\hat{H}_{\text{ex}} = -\sum_i h^\dagger_i h^i,$$

where in the U(1) slave boson representation,

$$\vec{S}_i \cdot \vec{h}_i = \frac{1}{2} \sum_{k=1}^{3} (c^\dagger_i \sigma^k_{\alpha \beta} c_i \sigma^k_{\alpha \beta}) h^k_i,$$

$$= \frac{1}{2} \sum_{k=1}^{3} (f^\dagger_i \sigma^k_{\alpha \beta} f^i h^k_i),$$

$$= \frac{1}{2} \sum_{k=1}^{3} (1 + b^\dagger_i b_i) (f^\dagger_i \sigma^k_{\alpha \beta} f^i h^k_i),$$

$$\simeq \frac{1}{2} \sum_{k=1}^{3} < (1 + b^\dagger_i b_i) > (f^\dagger_i \sigma^k_{\alpha \beta} f^i h^k_i),$$

(10)

The associated free energy is formally,

$$F = -\frac{1}{\beta} \ln Z,$$

(11)

where $\beta = 1/kT$ and the partition function,

$$Z = \int \mathcal{D}f \mathcal{D}b \mathcal{D}\chi \mathcal{D}\Delta \mathcal{D}^\dagger \mathcal{D}^\dagger \mathcal{D}\lambda e^{-\int_0^\tau dt L_{\text{eff}}}. $$

(12)

Converting the magnetic (spin) susceptibility,

$$\chi_{kk'}(\vec{r}_i - \vec{r}_j, \tau - \tau') = -\beta h \frac{\delta^2 F[\vec{h}]}{\delta h^k_i (\tau) \delta h^k_j (\tau')} \bigg|_{\vec{h}=0}. $$

(13)

into its four momentum space $(\vec{q}, \omega)$ expression and allowing isotropic response to the applied magnetic field, the RPA form of magnetic susceptibility is obtained to be,[23]

$$\chi(\vec{q}, \omega) = \frac{\chi^0(\vec{q}, \omega)}{1 + J(\vec{q})\chi^0(\vec{q}, \omega)}, $$

(14)
where \( f(\vec{q}) = 2f(\cos q_x + \cos q_y) \) and \( \chi^0(\vec{q}, \omega) \) is the irreducible magnetic susceptibility given by

\[
\chi^0(\vec{q}, \omega) = \frac{(1-x)^2}{4N} \sum_{\vec{q}'} \left\{ \begin{array}{c}
\left( E_{k+q}^f E_{k}^f + (\epsilon_{k+q}^f - \mu^f)(\epsilon_{k}^f - \mu^f) + \Delta_{k+q}^f \Delta_k^f \right) n^f(E_{k+q}^f) - n^f(E_k^f) \\
2E_{k+q}^f E_k^f \left( \frac{w - (E_{k+q}^f - E_k^f) + i\eta}{w - (E_{k+q}^f - E_k^f) + i\eta} \right) n^f(E_{k+q}^f) - n^f(-E_k^f) \\
2E_{k+q}^f E_k^f \left( \frac{w - (E_{k+q}^f - E_k^f) + i\eta}{w - (E_{k+q}^f - E_k^f) + i\eta} \right) n^f(-E_{k+q}^f) - n^f(E_k^f) \\
2E_{k+q}^f E_k^f \left( \frac{w - (E_{k+q}^f - E_k^f) + i\eta}{w - (E_{k+q}^f - E_k^f) + i\eta} \right) n^f(-E_{k+q}^f) - n^f(-E_k^f) \\
2E_{k}^f E_k^f \left( \frac{w - (E_{k+q}^f - E_k^f) + i\eta}{w - (E_{k+q}^f - E_k^f) + i\eta} \right) n^f(E_{k+q}^f) - n^f(-E_k^f) \end{array} \right\}
\]

(15)

where the quasi-spinon energy is \( E_k^f = \sqrt{(\epsilon_k^f - \mu^f)^2 + (\Delta_k^f)^2} \) with the effective bare spinon energy, \( \epsilon_k^f = -\frac{1}{2N}(\cos k_x + \cos k_y) - 4xt \cos k_x \cos k_y \); the spinon chemical potential, \( \mu^f \); the spinon gap, \( \Delta_k^f = \phi_k^s \Delta_k \); with \( \phi_k = \cos k_x - \cos k_y \) and \( n^f(E_k^f) = 1/(e^{E_k^f/T} + 1) \). In the complete expression of the effective Lagrangian Eq. 3, interplay between the two sectors, one for the spinon (spin) sector and the other for holon (charge) sector, namely Eq. 5 and Eq. 6 appears owing to the presence of coupling between the spinon pairing order and holon pairing order as shown in the last term of Eq. 6. Thus it should be noted that the effect of coupling between the two order parameter is embedded in the expression of the above irreducible magnetic susceptibility, Eq. 15, including the effect of the nearest neighbor hopping.

### 5. Computed results of magnetic susceptibility

Earlier, with the neglect of the next-nearest neighbor (or diagonal) hopping \( t' \) term we were able to obtain the generic feature of the dome shaped superconducting transition temperature and the monotonously decreasing pseudogap temperature in the phase diagram[5] in agreement with observations[15, 16]. Now with the inclusion of the diagonal hopping term, such generic feature is, still, well predicted in the computed result of the phase diagram as shown in Fig. 1 and Fig. 2. As a concerted study we use the predicted phase diagram shown in Fig. 3 to calculate the magnetic spin susceptibility of present interest. As in our earlier study of the magnetic susceptibility[21, 22], we take the negative value[7, 13] of the next-nearest neighbor hopping integral with the choice of \( t' = -0.45 \) (to conform with the study of Brinckmann and Lee[23]) in the \( t - t' - J \) Hamiltonian of interest[21].

In Fig. 4 we display the variation of magnetic susceptibility at \((\pi, \pi)\) with temperature T and transfer energy E at a fixed hole doping, \( x = 0.05 \). The magnetic resonance peak is shown to
Fig. 3. (color online) Phase diagram with $t'/t = -0.45$, $J/t = 0.5$. Both temperature $T$ and hole concentration $x$ are in reduced units, $T/t$ and $x/x_0$ respectively.

Fig. 4. (color online) Imaginary part of magnetic susceptibility vs. temperature and resonance energy at a fixed hole doping, $x = 0.05$ in the underdoped region decrease with increasing temperature and disappears at the onset temperature $T^*$. It shows a steady decrease of the resonance peak peak height with increasing temperature and eventual disappearance at $T^*$ in agreement with observation[17]. This indicates that the short-range AF spin fluctuations involved with the spin pairing correlations or the spin (spinon) singlet pairing order disappears at the onset temperature, $T^*$. He et al.[18] showed from their INS measurements of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) that in the underdoped cuprates the magnetic (spin) resonance peak energy $E_{\text{res}}$ (or $\omega_{\text{res}}$) increases with $T_c$ showing a linear scaling behavior between the two energy scales, $E_{\text{res}}$ and $T_c$, i.e., $E_{\text{res}}/T_c \simeq \text{const}$. In Fig. 5 we show that the predicted $E_{\text{res}}$ with $J_{\text{eff}} = \alpha J$ (where $\alpha = 0.4[23]$) monotonously increases with increasing $T_c$, yielding a linear scaling behavior of $E_{\text{res}}/T_c \simeq \text{const}$. This predicted linear scaling behavior is in agreement with the observations made by He et al.[18]. We note some quantitative differences between the observed value (around 5) and the predicted one (around 3).
6. Summary

In this study we applied the recently proposed slave-boson theory\[5\] in which the spin (spinon) paring order and the charge (holon) pairing order are coupled to result in the generic feature of the dome-shaped superconducting transition temperature and the monotonously decreasing spin gap temperature in the phase diagram. From the present study with the inclusion of the diagonal hopping $t'$ term we also found that such generic feature still holds, as shown in Fig. 1 through Fig. 3. Further we showed that there exists correlation (or interplay) between the two different temperature scales, $T^*$ and $T_C$, resulting in the increasing $T_C$ with increasing $T^*$. Relatedly, it can be said that the superconducting phase is correlated with the spin gap phase. We find that such correlation between the two phases is attributed to the short-range AF spin fluctuations involved with spin pairing correlations. The simultaneous increase of the superconducting transition temperature with the spin gap temperature with increasing $J$ is shown to be consistent with the observed phase diagrams for high $T_C$ cuprate samples (e.g., LSCO and BSCCO samples)\[15\] which shows that the higher $T^*$ samples always accompany higher $T_C$. In addition, to achieve a self-consistent, concerted study we used the predicted phase diagram to study the magnetic susceptibility. Specifically, resorting to the computed phase diagram shown in Fig. 3 we found that both the temperature dependence of the magnetic resonance peak and the linear scaling behavior of the magnetic (spin) resonance peak energy $E_{\text{res}}$ with the superconducting transition temperature $T_C$ agree with the INS measurements\[17, 18\]. We showed that this linear scaling behavior is attributed to the short-range AF spin fluctuations. Although not discussed here, such linear relation is found to be invariant with the Heisenberg coupling constant\[22\], implying high $T_C$ cuprate sample independence. In short, based on the above concerted studies of both the phase diagram and the magnetic susceptibility we find that the short-range (spin dimer) AF spin fluctuations of the shortest possible correlation length involved with the spin pairing correlations are responsible for high $T_C$ superconductivity. We argue that this finding is supported by the reproducibility of both the dome-shaped superconducting transition temperature, $T_C$ in the phase diagram and the linear scaling behavior between $E_{\text{res}}$ and $T_C$, in both of which the $T_C$
and thus the superconducting phase transition is shown to occur as a result of the short-range AF spin fluctuations in association with the spin-charge coupling.

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8. Appendix A: Heisenberg interaction term in the U(1) slave-boson representation

The t-J Hamiltonian of interest is given by,

\[
H = -t \sum_{<ij>} (\epsilon_{iv}^i \epsilon_{jv}^j + c.c.) + J \sum_{<ij>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \\
- \mu \sum_i \epsilon_{iv}^i c_{iv}^\dagger c_{iv}
\]  

(A1)

and the Heisenberg interaction term is rewritten

\[
H_{J} = J \sum_{<ij>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \\
= \frac{J}{2} \sum_{<ij>} (c_{iv}^i c_{jv}^j - c_{iv}^j c_{jv}^i)(c_{iv}^i c_{jv}^j - c_{iv}^j c_{jv}^i).
\]  

(A2)

Here \(t\) is the hopping energy and \(S_i\), the electron spin operator at site \(i\); \(S_i \cdot \frac{\sigma_{i\alpha}}{2} \cdot \sigma_{i\beta} = c_{i\alpha}^\dagger c_{i\beta}\) with \(\sigma_{\alpha\beta}\), the Pauli spin matrix element. \(n_i\) is the electron number operator at site \(i\), \(n_i = c_{i\alpha}^\dagger c_{i\alpha}\). \(\mu\) is the chemical potential.

In the U(1) slave-boson representation[1, 2, 24, 25], with single occupancy constraint at site \(i\) the electron annihilation operator \(c_{iv}\) is taken as a composite operator of the spinon (neutral charged fermion) annihilation operator \(f_{iv}\) and the holon (positively charged boson) creation operator \(b_{iv}^\dagger\), and thus, \(c_{iv} = f_{iv} b_{iv}^\dagger\). Rigorously speaking, it should be noted that the expression \(c_{iv} = b_{iv}^\dagger f_{iv}\) is not precise since these operators belong to different Hilbert spaces and thus the equality sign here should be taken only as a symbol for mapping. Using \(c_{iv} = f_{iv} b_{iv}^\dagger\) and introducing the Lagrange multiplier term (the last term in Eq.(A3)) to enforce single occupancy constraint, the t-J Hamiltonian is rewritten,

\[
H = -t \sum_{<ij>} (f_{iv}^i b_{iv}^j) (b_{iv}^\dagger f_{jv}^j + c.c.) + H_j \\
- \mu \sum_i f_{iv}^i b_{iv}^\dagger f_{iv}^\dagger b_{iv}^\dagger \\
- i \sum \lambda_i (b_{iv}^\dagger b_{iv} + f_{iv}^\dagger f_{iv} - 1)
\]  

(A3)
with the Heisenberg interaction term,

$$H_J = -\frac{J}{2} \sum_{<i,j>} b_i b_j b_i^\dagger b_j^\dagger (f_i^\dagger f_j^\dagger f_i f_j - f_i^\dagger f_j^\dagger f_j f_i).$$  \hfill (A4)

The first term represents hopping of a spinon from site \( i \) to site \( j \) and of a holon (positively charged boson) from site \( i \) to site \( j \). In the slave-boson representation a charged fermion (electron or hole) is taken as a composite particle of a ‘spinon’ and a ‘holon’. They can conveniently serve as book-keeping labels to discern physical properties or objects involved with the charge or spin degree of freedom (e.g., spin gap phase, spin singlet pairs, hole pairs, ...). With the single occupancy constraint, electron is allowed to hop from a singly occupied copper site \( i \) only to a vacant copper site \( j \). A site of single occupancy in the \( CuO_2 \) plane of high \( T_c \) cuprates physically represents an electrically neutral site (net charge 0) with an electron of spin \( 1/2 \) and the vacant site, a site of positive charge +e with net spin 0. In the slave-boson representation, hopping of an electron (a composite of spinon and holon) from a singly occupied copper site (neutral site) \( j \) to an empty site (positively charged site with +e) \( i \) results in the annihilation of a spinon (a fermion of charge 0 and spin 1/2) and the creation of a positively charged holon (a boson of charge +e and spin 0) at site \( j \) while at the copper site \( i \) a composite of a spinon (fermion of charge 0 and spin 1/2) and a negatively charged holon is created. It is of note that as a result of electron hopping the newly occupied copper site \( i \) in the \( CuO_2 \) plane can, also, be labeled as ‘spinon’ since this is an electrically neutral (charge 0) site with an electron of spin 1/2 and the vacant site \( j \), a site of positive charge +e and spin 0 as mentioned above. Thus in practical sense, there is no distinction between the two different cases above. At times, we will call the singly occupied site as ‘spinon’ and the vacant (empty) site as ‘holon’ as long as there is no confusion. This is because any site occupied by a spinon is identified as an electrically neutral site occupied by a single electron with spin 1/2 and the site with a positive holon is a positively charged vacant site with spin 0. Thus physical spin-charge separation is not allowed.

The Heisenberg interaction term, Eq.(A4) shows coupling between the charge and spin degrees of freedom. Physics involved with the charge degree of freedom is manifested by the four holon (boson) operator \( b_i b_j b_j^\dagger b_i^\dagger \) in the Heisenberg interaction term. Judging from the intersite charge coupling term \( \frac{1}{4} n_i n_j \) present in the Heisenberg interaction term \( H_I = J \sum_{<i,j>} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \), it is obvious that this charge contribution can not be neglected in its slave-boson representation. It is to be noted that the Hubbard Hamiltonian contains repulsive interaction \( U \) between charged particles and is mapped into the t-J Hamiltonian \( H_{t-J} \) in the large \( U \) limit. The Coulomb repulsion, \( U n_{i\uparrow} n_{i\downarrow} = \frac{U}{4} (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{4} (n_{i\uparrow} - n_{i\downarrow})^2 \) obviously manifests the presence of both the charge (the first term) and spin (the second term) degrees of freedom. Thus, under mapping the charge part of contribution naturally appears in the Heisenberg interaction term.

Let us now take another look at the importance of the charge contribution. In general, uncertainty principle between the number density (amplitude) and the phase of a boson order parameter applies. As an example, arbitrarily large fluctuations of the number density fix the phase, or arbitrarily large phase fluctuations fix the number density of the boson.
conventional BCS superconductors of long coherence length meet the former classification, and thus the phase fluctuations of the Cooper pair order parameter are minimal. For charged bosons, e.g., the Cooper pairs, the number density fluctuations refer to charge density fluctuations. For short coherence length superconductors such as the high $T_c$ cuprate systems of present interest, local charge density fluctuations exist and cause large phase fluctuations. Thus, both the charge and phase fluctuations need to be taken into account to fully exploit the quantum fluctuations.

Let us now consider the importance of the charge and spin fluctuations. In generally, coupling between physical quantities $A$ and $B$ is decomposed into terms involving fluctuations of $A$, i.e., $(A - < A >)$ and $B$, i.e., $(B - < B >)$, separately uncorrelated mean field contribution of $< A >$ and $< B >$ and correlation between fluctuations of $A$ and $B$, that is, $(A - < A >)$ and $(B - < B >)$ respectively; $AB = (A - < A >)(B - < B >) + (A - < A >)(B - < B >) + (A - < A >)(B - < B >)$. Setting $A = b_i b^\dagger_i$ for charge (holon) contribution and $B = (f^\dagger_i f_i) - (f^\dagger_i f_i)$ for spin (spinon) contribution, the Heisenberg coupling term, Eq(A4) can be decomposed into terms involving coupling between the charge and spin fluctuations separately, the mean field contributions and coupling (correlation) between fluctuations (charge and spin fluctuations). Using such decomposition of the Heisenberg interaction term for Eq.(A3), we write the partition function,

$$Z = \int DbDf_iD\lambda e^{-S[b,f,\lambda]},$$

where

$$S[b,f,\lambda] = \int_0^\beta d\tau \left[ \sum_i b_i^\dagger \partial_\tau b_i + \sum_i f_i^\dagger \partial_\tau f_i + H^{U(1)}_{t \rightarrow i} \right]$$

with $\beta = \frac{1}{k_B T}$, the inverse temperature and $H^{U(1)}_{t \rightarrow i}$, the U(1) symmetry preserved Hamiltonian,

$$H^{U(1)}_{t \rightarrow i} = -t \sum_{<i,j>} \left( f_{i \sigma}^\dagger f_{j \sigma} b_i^\dagger b_j + c.c. \right)$$

$$- \sum_{<i,j>} \left[ \left( f_{i \sigma}^\dagger f_{j \sigma}^\dagger - f_{i \sigma}^\dagger f_{j \sigma} \right) \left( f_{j \sigma} f_{i \sigma} - f_{j \sigma} f_{i \sigma}^\dagger \right) \right] b_i b_j^\dagger b_j$$

$$+ \left( f_{i \sigma}^\dagger f_{j \sigma} - f_{i \sigma} f_{j \sigma}^\dagger \right) \left( f_{j \sigma}^\dagger f_{i \sigma} - f_{j \sigma} f_{i \sigma} \right)$$

$$+ \left( f_{i \sigma}^\dagger f_{j \sigma} - f_{i \sigma} f_{j \sigma}^\dagger \right) \left( f_{j \sigma}^\dagger f_{i \sigma} - f_{j \sigma} f_{i \sigma} \right)$$

$$+ \left( f_{i \sigma}^\dagger f_{j \sigma} - f_{i \sigma} f_{j \sigma}^\dagger \right) \left( f_{j \sigma}^\dagger f_{i \sigma} - f_{j \sigma} f_{i \sigma} \right)$$

$$- \left( f_{i \sigma}^\dagger f_{j \sigma}^\dagger - f_{i \sigma}^\dagger f_{j \sigma} \right) \left( f_{j \sigma}^\dagger f_{i \sigma} - f_{j \sigma} f_{i \sigma} \right)$$

$$- \sum_i f_{i \sigma}^\dagger f_{i \sigma} (1 + b_i^\dagger b_i + \lambda_i) (f_{i \sigma} f_{i \sigma}^\dagger + b_i^\dagger b_i - 1).$$

(7)
8.1 U(1) mean field Hamiltonian

Noting that $[b_i, b_j^\dagger] = \delta_{ij}$ for boson, the intersite charge (holon) interaction term (the second term) in Eq.(A7) is rewritten,

$$-\frac{J_p}{2} \left< (f_{i\uparrow}^\dagger f_{j\uparrow}^\dagger - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{i\downarrow} f_{i\downarrow} - f_{i\downarrow} f_{i\downarrow}) \right> b_i b_j b_i^\dagger b_j^\dagger$$

$$= -\frac{J_p}{2} < |\Delta_{ij}^f|^2 >^2 \left( 1 + b_i^\dagger b_i + b_j^\dagger b_j + b_i^\dagger b_j b_j^\dagger b_i \right),$$  

(A8)

with $\Delta_{ij}^f = f_{i\uparrow} f_{j\downarrow} - f_{j\downarrow} f_{i\uparrow}$, the spinon pairing field. The third term in Eq.(A7) represents the intersite spin (spinon) interaction and is rewritten,

$$-\frac{J_p}{2} \left< b_i b_j b_i^\dagger b_j^\dagger \right> (f_{i\uparrow}^\dagger f_{j\uparrow}^\dagger - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{i\downarrow} f_{i\downarrow} - f_{i\downarrow} f_{i\downarrow})$$

$$= -\frac{J_p}{2} (f_{i\uparrow}^\dagger f_{j\uparrow} - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{i\downarrow} f_{i\downarrow} - f_{i\downarrow} f_{i\downarrow}),$$  

(A9)

where $J_p = J(1 + < b_i^\dagger b_i > + < b_j^\dagger b_j > + < b_i^\dagger b_j b_j^\dagger b_i >)$ or $J_p = J(1 - x)^2$ with $x$, the uniform hole doping concentration[27]. The fourth term in Eq.(A7) is written,

$$\frac{J_p}{2} \left< b_i b_j b_i^\dagger b_j^\dagger \right> (f_{i\uparrow}^\dagger f_{j\uparrow}^\dagger - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{i\downarrow} f_{i\downarrow} - f_{i\downarrow} f_{i\downarrow})$$

$$= \frac{J_p}{2} \left( 1 + < b_i^\dagger b_i > + < b_j^\dagger b_j > + < b_i^\dagger b_j b_j^\dagger b_i > \right) < |\Delta_{ij}^f|^2 > .$$  

(A10)

The intersite spinon interaction term in Eq.(A9) is decomposed into the direct, exchange and pairing channels[25],

$$-\frac{J_p}{2} (f_{i\uparrow}^\dagger f_{j\uparrow} - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{i\downarrow} f_{i\downarrow} - f_{i\downarrow} f_{i\downarrow})$$

$$= \frac{J_p}{4} \sum_{k=1}^{3} \left( f_{i\alpha}^\dagger \sigma_{\alpha \beta}^k f_{j\beta}^\dagger (f_{j\uparrow}^\dagger \sigma_{\uparrow \downarrow}^k f_{i\downarrow}^\dagger) - (f_{i\alpha}^\dagger \sigma_{\alpha \beta}^k f_{j\beta}) (f_{j\uparrow}^\dagger \sigma_{\uparrow \downarrow}^k f_{i\downarrow}^\dagger) \right)$$

$$= v_D + v_E + v_P,$$  

(A11)

with $\sigma^0 = I$, the identity matrix and $\sigma^{1,2,3}$, the Pauli spin matrices, where $v_D$, $v_E$ and $v_P$ are the spinon interaction terms of the direct, exchange and pairing channels respectively,

$$v_D = -\frac{J_p}{8} \sum_{k=0}^{3} (f_{i\alpha}^\dagger \sigma_{\alpha \beta}^k f_{j\beta}^\dagger) (f_{j\uparrow}^\dagger \sigma_{\uparrow \downarrow}^k f_{i\downarrow}^\dagger),$$  

(A12)

$$v_E = -\frac{J_p}{4} \left( (f_{i\alpha}^\dagger f_{j\beta}^\dagger)(f_{j\uparrow}^\dagger f_{i\downarrow}^\dagger) - n_i \right),$$  

(A13)

$$v_P = -\frac{J_p}{2} (f_{i\uparrow}^\dagger f_{j\uparrow} - f_{i\uparrow}^\dagger f_{j\uparrow})(f_{j\downarrow} f_{i\downarrow} - f_{j\downarrow} f_{i\downarrow}).$$  

(A14)

Here $\sigma^0$ is the unit matrix and $\sigma^{1,2,3}$, the Pauli spin matrices.
Combining Eq.(A8) and Eq.(A10), we have

\[ \frac{1}{2} < |\Delta_{ij}^f|^2 > \left( 1 + b_i^\dagger b_i + b_j^\dagger b_j + b_i^\dagger b_j b_j^\dagger b_i^\dagger \right) \]

\[ + \frac{1}{2} < |\Delta_{ij}^f|^2 > \left( 1 + b_i^\dagger b_i + b_j^\dagger b_j + b_i^\dagger b_j b_j^\dagger b_i^\dagger \right) \]

\[ = \frac{1}{2} < |\Delta_{ij}^f|^2 > b_i^\dagger b_i b_i^\dagger b_i + \frac{1}{2} < |\Delta_{ij}^f|^2 > b_i^\dagger b_i b_i^\dagger b_i > \]

\[ - \frac{1}{2} < |\Delta_{ij}^f|^2 > \left( \left( b_i^\dagger b_i + b_j^\dagger b_j > b_i^\dagger b_j b_j^\dagger b_i^\dagger \right) \right). \tag{A15} \]

Collecting the decomposed terms Eq.(A8) through Eq.(A10) in association with Eqs.(A11) through Eq.(A15), we write

\[ H_f = -\frac{1}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 b_i^\dagger b_j b_j^\dagger b_i \]

\[ - J_p \sum_{<ij>} \left[ \frac{1}{2} (f_i^\dagger f_i - f_i f_i^\dagger) (f_j^\dagger f_j - f_j f_j^\dagger) \right] \]

\[ + \frac{1}{4} \left( (f_{\sigma i}^\dagger f_{\sigma i})(f_{\sigma j}^\dagger f_{\sigma j}) - n_i \right) \]

\[ + \frac{1}{8} \sum_{\kappa=\uparrow,\downarrow} (f_{\kappa i}^\dagger \sigma^k f_{\kappa i})(f_{\kappa j}^\dagger \sigma^k f_{\kappa j}) \]

\[ + \frac{1}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 < b_i^\dagger b_i > < b_j^\dagger b_j > \]

\[ - \frac{1}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 \left[ \left( b_i^\dagger b_i + b_j^\dagger b_j > b_i^\dagger b_j b_j^\dagger b_i^\dagger \right) \right], \tag{A16} \]

where we considered \( < |\Delta_{ij}^f|^2 > |\Delta_{ij}^f|^2 \) and ignored the fifth term in Eq.(A7).

Hubbard Stratonovich transformation for the holon pairing term (the second term of Eq.(A16)) leads to

\[ \frac{\alpha}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 b_i^\dagger b_j b_j^\dagger b_i \alpha \int \prod_{<ij>} d\Delta_{ij}^f d\Delta_{ij}^{f\dagger} - \frac{\alpha}{2} \sum_{<ij>} \left[ |\Delta_{ij}^f|^2 - \Delta_{ij}^{f\dagger}(b_i b_j) - \Delta_{ij}^f (b_i^\dagger b_j^\dagger) \right] \tag{A17} \]

and the saddle point approximation yields,

\[ H^b_f = \sum_{<ij>} \frac{1}{2} |\Delta_{ij}^f|^2 \left[ |\Delta_{ij}^{0b}|^2 - \Delta_{ij}^{0b}(b_i b_j) - \Delta_{ij}^b (b_i^\dagger b_j^\dagger) \right], \tag{A18} \]

where \( \Delta_{ij}^{0b} = < b_i b_j > \) is the saddle point for the holon pairing order parameter \( \Delta_{ij}^b \). Since confusion is not likely to occur, we will use the notation \( \Delta_{ij}^b \) in place of \( \Delta_{ij}^{0b} \) for the saddle point. As are shown in Eqs.(A12) through (A14) the spinon interaction term is decomposed into the direct, exchange and pairing channels respectively. Proper Hubbard-Stratonovich

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transformation corresponding to these channels and saddle point approximation leads to the effective Hamiltonian,

\[
H_{\text{eff}} = \frac{J_p}{4} \sum_{<ij>} \left[ |\chi_{ij}|^2 - \chi_{ij}^* (f_{i\sigma}^\dagger f_{j\sigma} + \frac{4J}{J_p} b_{i\uparrow}^\dagger b_{j\downarrow}) - \text{c.c.} \right]
\]

\[
+ \frac{J_p}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 \left[ |\Delta_{ij}^b|^2 - \Delta_{ij}^{b+} (b_{i\uparrow} b_{j\downarrow}) - \text{c.c.} \right]
\]

\[
+ \frac{J_p}{2} \sum_{<ij>} \left[ |\Delta_{ij}^f|^2 - \Delta_{ij}^f (f_{i\uparrow}^\dagger f_{j\uparrow} - f_{i\downarrow}^\dagger f_{j\downarrow}) - \text{c.c.} \right]
\]

\[
+ \frac{J_p}{2} \sum_{<ij>} \left[ (\rho_l^i)^2 - \rho_l^i (f_{i\sigma}^\dagger v_l^i f_{j\sigma}) \right] + \frac{J_p}{2} \sum_i (f_{i\sigma}^\dagger f_{i\sigma})
\]

\[
+ \frac{4J^2}{J_p} \sum_{<ij>} (b_{i\uparrow} b_{j\uparrow})(b_{i\downarrow} b_{j\downarrow})
\]

\[
+ \frac{J_p}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 < b_{i\uparrow} b_{j\downarrow} > < b_{i\downarrow} b_{j\uparrow} >
\]

\[
- \frac{J_p}{2} \sum_{<ij>} |\Delta_{ij}^f|^2 \left[ (b_{i\uparrow} b_{j\downarrow} - < b_{i\uparrow} b_{j\downarrow} >) + (b_{i\downarrow} b_{j\uparrow} - < b_{i\downarrow} b_{j\uparrow} >) \right]
\]

\[
- \mu \sum_i f_{i\sigma}^\dagger f_{i\sigma} (1 + b_{i\uparrow} b_{i\downarrow}) - i \sum_i \lambda_i (f_{i\sigma}^\dagger f_{i\sigma} + b_{i\uparrow} b_{i\downarrow} - 1),
\]

where \(\Delta_{ij}^b = < b_{i\uparrow} b_{j\downarrow} >, \chi_{ij} = < f_{i\sigma}^\dagger f_{j\sigma} + \frac{4J}{J_p} b_{i\uparrow} b_{j\downarrow} >, \Delta_{ij}^f = < f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} > \) and \(\rho_l^i = \frac{1}{2} f_{i\sigma}^\dagger v_l^i f_{i\sigma} \)

are proper saddle points.

We note that \(\rho_l^i = \frac{1}{2} f_{i\sigma}^\dagger v_l^i f_{i\sigma} \) and \(\rho_l^0 = \frac{1}{2} < f_{i\sigma}^\dagger f_{i\sigma} > \) for \(l = 0 \) for the contribution of the direct spinon interaction term (the fourth term). The expression \((b_{i\uparrow} b_{j\downarrow})(b_{i\downarrow} b_{j\uparrow})\) in the fifth term of Eq.(A19) represents the exchange interaction channel. The exchange channel will be ignored owing to a large cost in energy, \(U \approx \frac{4J^2}{J_p} [25, 26] \). The resulting effective Hamiltonian is

\[
H^{MF} = H^{\Delta \chi} + H^b + H^f,
\]

where \(H^{\Delta \chi} \) represents the the saddle point energy involved with the spin pairing order parameter \(\Delta^f\), the holon pairing order parameter \(\Delta^b\) and the hopping order parameter \(\chi\),

\[
H^{\Delta \chi} = \sum_{<ij>} \left[ \frac{1}{2} |\Delta_{ij}^f|^2 |\Delta_{ij}^b|^2 + \frac{1}{2} |\Delta_{ij}^f|^2 \chi^2 \right]
\]

\[
+ \frac{J_p}{2} \sum_{<ij>} \left[ |\Delta_{ij}^f|^2 + \frac{1}{2} |\chi_{ij}|^2 + \frac{1}{4} \right].
\]
$H^b$ is the holon Hamiltonian,

$$
H^b = -t \sum_{<ij>} \left[ \chi^*_{ij}(b_i^†b_j) + \text{c.c.} \right] - \sum_{<ij>} \frac{J_p}{2} |\Delta_f|^2 \left[ \Delta^b_{ij} (b_i b_j) + \text{c.c.} \right] - \sum_i \mu^b_i (b_i^†b_i - x),
$$

(A22)

where $\mu^b_i = i\lambda_i + \frac{1}{2} \sum_{j=\pm x, \pm y} |\Delta_f|^2$ and $H^f$, the spinon Hamiltonian,

$$
H^f = -\frac{J_p}{4} \sum_{<ij>} \left[ \chi^*_{ij}(f_i^†f_j) + \text{c.c.} \right] - \frac{J_p}{2} \sum_{<ij>} \left[ \Delta^f_{ij} (f_i^†f_j - f_j^†f_i) + \text{c.c.} \right] - \sum_i \mu^f_i (f_i^†f_i - (1 - x)),
$$

(A23)

where $\mu^f_i = \mu(1 - x) + i\lambda_i$.

As can be seen from Eqs.(A21) through (A23), Eq.(A20) reveals the importance of coupling between the spin and charge degrees of freedom, that is, coupling between the spinon pairing and holon pairing. Thus no spin-charge separation appears in the mean-field Hamiltonian above contrary to other mean field theories[1–3, 24, 26] which pay attention to the single-holon bose condensation. As can be seen from the second term in Eq.(A22) which represents holon pairing contribution it is expected that, owing to the coupling effect, bose condensation (or superconducting phase transition) will occur only in the presence of the non-vanishing spin singlet pairing order, $\Delta_f$ owing to the coupling effects mentioned above. Indeed, in high $T_c$ cuprates superconductivity is not observed above the pseudogap (spin gap) temperatures $T^*$ where the spin singlet pairing order disappears.

### 8.2 U(1) free energy

The diagonalized Hamiltonian for Eq.(A20) above is obtained to be (see Appendix A for detailed derivations),

$$
H_{MF}^{U(1)} = NJ \left[ \Delta^2_\alpha + \Delta^2_\beta \right] + N J_p \left[ \Delta^2_\gamma + \frac{1}{2} \lambda^2 + \frac{1}{4} \right]
$$

$$
+ \sum_{k,s} E_{ks}^f (a_{ks\uparrow}^†a_{ks\uparrow} - a_{ks\downarrow}^†a_{ks\downarrow}) - N x \mu^f
$$

$$
+ \sum_{k,s=\pm 1} E_{ks}^h (\beta_{ks\uparrow}\beta_{ks\uparrow} + \frac{1}{2} (E_{ks}^b + \mu^b) + \mu^b N x,
$$

(A24)

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where $E_{ks}^{\alpha}$ is the quasispinon excitation energy,

$$E_{ks}^{\alpha} = \sqrt{(\epsilon_{ks}^{\alpha} - \mu)^2 + (\Delta_0^\alpha)^2}$$  \hspace{1cm} (A25)

with the spinon pairing energy (gap), $\Delta_0^\alpha = J_f \zeta_k (\tau^\alpha \Delta_f)$, and $E_{ks}^{b \beta}$ is the quasiholon excitation energy,

$$E_{ks}^{b \beta} = \sqrt{(\epsilon_{ks}^{b \beta} - \mu)^2 - (\Delta_0^\beta)^2},$$  \hspace{1cm} (A26)

where the holon pairing energy, $\Delta_0^\beta = J_b \Delta_b (\tau^b \Delta_b)$ and with $\phi = \theta, \tau^\alpha$ or $\tau^b$,

$$\zeta_k (\phi) = \sqrt{\gamma_k^2 \cos^2 \phi + q_k^2 \sin^2 \phi},$$  \hspace{1cm} (A27)

$$\epsilon_{ks}^{\alpha} = \frac{I_p}{2} s \chi_{kk} (\theta),$$  \hspace{1cm} (A28)

$$\epsilon_{ks}^{b \beta} = 2 t s \chi_{kk} (\theta),$$  \hspace{1cm} (A29)

with $\gamma_k = (\cos k_x + \cos k_y)$ and $q_k = (\cos k_x - \cos k_y)$. $\sum'$ denotes the summation over momentum $k$ in the half reduced Brillouin zone, and $s = +1$ and $-1$ represent the upper and lower energy bands of quasiparticles respectively. Here $a_{ks \uparrow} (a_{ks \uparrow}^\dagger)$ and $a_{ks \downarrow} (a_{ks \downarrow}^\dagger)$ are the annihilation(creation) operators of spinon quasiparticles of spin up and spin down respectively, and $\beta_{ks} (\beta_{ks}^\dagger)$, the annihilation(creation) operators of holon quasiparticles of spin 0. $\epsilon_{ks}^{\alpha}$ and $\epsilon_{ks}^{b \beta}$ are the kinetic energies for spinons and holons respectively. The minus sign $(-\Delta^2)$ in the expression of the holon quasiparticle energy $\sqrt{(\epsilon - \mu)^2 - \Delta^2}$ arises as a consequence of the Bose Einstein statistics[28]. From the diagonalized Hamiltonian Eq.(A24), we calculate the total free energy.

Rewriting Eq.(A24) as

$$H_{U(1)}^{MF} = \sum_{k,s=\pm 1} \left[ E_{ks}^{\alpha} (a_{ks \uparrow}^\dagger a_{ks \uparrow} - a_{ks \downarrow} a_{ks \downarrow}^\dagger) + E_{ks}^{b \beta} \beta_{ks}^\dagger \beta_{ks} \right]$$  \hspace{1cm} (A30)

with

$$H_c = NJ \Delta_b^2 (\Delta_b^2 + x^2) + N J_p (\Delta_f^2 + \frac{x^2}{2} + \frac{1}{4})$$

$$+ \sum_{k,s=\pm 1} \frac{E_{ks}^{b \beta} + \mu}{2} - N x \mu^f + N x \mu^b,$$  \hspace{1cm} (A31)

the partition function is derived to be,

$$Z = \exp (-\beta H_c) \prod_{k,s=\pm 1} (2 \cosh \frac{\beta E_{ks}^{\alpha}}{2})^2 (1 - e^{-\beta E_{ks}^{b \beta}})^{-1}.$$  \hspace{1cm} (A32)
Using the above expression, the total free energy is given by

\[
F(U) = NJ^2 \left( \Delta_b^2 + x^2 \right) + NJ^2 \left( \Delta_f^2 + \frac{x^2}{4} + \frac{1}{4} \right)
\]

\[
- 2k_B T \sum_{k,s=\pm 1} \ln(\cosh(\beta E_{k,s}^f/2)) - N\chi_f^2 - 2Nk_B T \ln 2
\]

\[
+ k_B T \sum_{k,s=\pm 1} \ln(1 - e^{-\beta E_{k,s}^b}) + \sum_{k,s=\pm 1} \frac{E_{k,s}^b + \mu^b}{2} + N\chi_b^2.
\]

(A33)

The set of uniform phase \((\theta = 0)\) for the hopping order parameter, d-wave symmetry \((\tau^d = \pi/2)\) for the spinon pairing order parameter and s-wave symmetry \((\tau^s = 0)\) for the holon pairing order parameter is found to yield a stable saddle point energy for both the underdoped and overdoped regions. There is another set of order parameters which yield the same energy as the above one; 2π-flux phase \((\theta = \pi/2)\) for the hopping order parameter, s-wave symmetry \((\tau^s = \pi/2)\) for the spinon pairing order parameter and d-wave symmetry \((\tau^d = 0)\) for the holon pairing order parameter. In both cases, the d-wave symmetry of the electron or hole (not holon) pairs occurs as a composite of the d-wave (s-wave) symmetry of spinon pairs and s-wave (d-wave) symmetry of holon pairs. Only at very low doping near half filling, the flux phase\([25]\) becomes more stable. Thus, the phase of the order parameters of present interest are \(\theta = 0, \tau^d = \pi/2\) and \(\tau^s = 0\). Then the d-wave symmetry of the electron or hole (not holon) pairs is a composite of the d-wave symmetry of spinon pairs and s-wave symmetry of holon pairs. Minimizing the free energy with respect to the amplitudes of the order parameters \(\chi\), \(\Delta_b\) and \(\Delta_f\), we obtain the self-consistent equations for the order parameters,

\[
\frac{\partial F(U)}{\partial \chi} = NJ f \chi - \sum_{k,s} \left( \tanh \frac{\beta E_{k,s}^f}{2} \right) \left( \frac{\partial E_{k,s}^f}{\partial \chi} \right) = 0,
\]

(A34)

\[
\frac{\partial F(U)}{\partial \Delta_b} = 2N J \Delta_b \Delta_b
\]

\[
+ \sum_{k,s} \left( \frac{1}{e^{\beta E_{k,s}^b} - 1} + \frac{1}{2} \right) \left( \frac{\partial E_{k,s}^b}{\partial \Delta_b} \right) = 0,
\]

(A35)

\[
\frac{\partial F(U)}{\partial \Delta_f} = 2N J \Delta_f + 2N J (\Delta_b^2 + x^2)
\]

\[
- \sum_{k,s} \left( \tanh \frac{\beta E_{k,s}^f}{2} \right) \left( \frac{\partial E_{k,s}^f}{\partial \Delta_f} \right) = 0.
\]

(A36)
For fixed numbers of spinon and holon at a given hole concentration, we obtain, for the chemical potentials, $\mu^f$ and $\mu^b$,

$$\frac{\partial F_{U(1)}}{\partial \mu^f} = \sum_{k,s=\pm 1}^i \left( \tanh \frac{\beta E_{ks}^f}{2} \right) \left( \frac{e_{ks}^f - \mu^f}{E_{ks}^f} \right) - Nx = 0, \quad \text{(A37)}$$

$$\frac{\partial F_{U(1)}}{\partial \mu^b} = -\sum_{k,s=\pm 1}^i \frac{1}{e^{\beta E_{ks}^b} - 1} \frac{e_{ks}^b - \mu^b}{E_{ks}^b} + \frac{e_{ks}^b - \mu^b - E_{ks}^b}{2E_{ks}^b} + Nx = 0. \quad \text{(A38)}$$

Using the five self-consistent equations of Eqs.(A34) through (A38), we determine $\chi$, $\Delta^b$, $\Delta^f$, $\mu^f$, and $\mu^b$ at each doping and temperature. Both the pseudogap temperature $T^*$ and the superconducting transition (boson condensation) temperature $T_c$ are determined to be the temperatures at which the spin gap $\Delta^f_0$ and the holon pairing energy (gap) $\Delta^b_0$ respectively begin to open.

**Appendix B: SU(2) action from the U(1) action**

The t-J Hamiltonian is manifestly invariant under the local SU(2) transformation $g_i = e^{i\sigma \cdot \theta}$ for both the spinon and holon spinors with

$$ \begin{pmatrix} f_{i1}^\dagger \\ f_{i2}^\dagger \end{pmatrix} = g_i \begin{pmatrix} f_{i1}^\dagger \\ f_{i2}^\dagger \end{pmatrix}, \quad \begin{pmatrix} f_{i1} \\ f_{i2} \end{pmatrix} = g_i \begin{pmatrix} f_{i1} \\ f_{i2} \end{pmatrix}$$

and

$$ \begin{pmatrix} b_{i1} \\ b_{i2} \end{pmatrix} = g_i \begin{pmatrix} b_{i1} \\ b_{i2} \end{pmatrix}, \quad \begin{pmatrix} b_{i1} \\ b_{i2} \end{pmatrix} = g_i \begin{pmatrix} b_{i1} \\ b_{i2} \end{pmatrix}. $$

We introduce additional Lagrange multiplier terms involved with the constraints $f_{i1}f_{i1} = 0$ and $f_{i1}f_{i1} = 0$ to write

$$-i \sum_i \lambda_i (f_{i1}^\dagger f_{i1} + b_{i1}^\dagger b_{i1} - 1) - i \sum_i \lambda_i f_{i1}^\dagger f_{i1} - i \sum_i \lambda_i f_{i1} f_{i1}$$

in order to allow for SU(2) symmetry. Thus writing spinors $\psi^0_{i1} = \begin{pmatrix} f_{i1}^\dagger \\ f_{i1} \end{pmatrix}$ and $\psi^0_{i2} = \begin{pmatrix} f_{i1} \\ -f_{i1}^\dagger \end{pmatrix}$ for spinon, $b^0_{i1} = \begin{pmatrix} b_{i1} \\ 0 \end{pmatrix}$ for holon and the three-component Lagrangian multiplier field $a^i_0$ with $a^{0(1)}_i = i\lambda^i_1 + i\lambda^d_1$, $a^{0(2)}_i = -\lambda^i_1 + \lambda^d_1$, $a^{0(3)}_i = i\lambda^i_1$, the U(1) action in Eq.(A6) can be rewritten as
\[ S_{U(1)}[b,f,a] = \int_0^\beta d\tau \left[ \sum_i \hbar^{0t}_i \partial_\tau \hbar^0_i + \frac{1}{2} \sum_{i,a} \psi'^{0t}_{ia} \partial_\tau \psi^0_{ia} - t \sum_{<ij>} \left( \left( \psi'^{0t}_{ia} \hbar^0_j \right) \left( \psi^0_{ia} \hbar^0_j \right) \right) + \text{c.c.} \right] \]

\[-\frac{1}{2} \sum_{<ij>} \hbar^{0t}_i \hbar^{0t}_j \hbar^{0t}_i \hbar^{0t}_j (f^+_if^+_j - f'^+_if'^+_j)(f^-if^-j - f'^-_if'^-_j) \]

\[-\mu \sum_i f^+_if^-i (b^+_i b^-_i + 1) - \sum_i \alpha^0_i \left( \frac{1}{2} \psi'^{0t}_{ia} \sigma \psi^0_{ia} + \hbar^{0t}_i \hbar^{0t}_i \right) \]  

where \( H \) is the fourth term is the Heisenberg interaction term, \( H_j = -\frac{1}{2} \sum_{<ij>} \hbar_i \hbar_j \hbar_i \hbar_j (f^+_if^+_j - f'^+_if'^-_j)(f^-if^-j - f'^-_if'^-_j) \).

We rewrite the spinon part of the Heisenberg interaction,

\[-\frac{1}{2} (f^+_if^+_i - f'^-_if'^-_i)(f^-if^-i - f'^-_if'^-_i) \]

\[ = \frac{1}{4} \sum_{k=1}^3 (f^+_i f^+_i f^+_i f^+_i)(f^-if^-i)(f^+_if^+_i)(f^-if^-i) \]

\[ = \frac{1}{4} \left[ \left( \Psi^0_i \Psi^0_i \left( \sigma^k \right)^T \right) \left( \Psi^0_i \Psi^0_i \left( \sigma^k \right)^T \right) - \left( f^+_i f^+_i f^+_i f^+_i \right) \right] \]  

\[ \Psi^0_i \equiv \left( f^+_i f^+_i f^+_i f^+_i \right) \] and \( (f^+_i f^+_i f^+_i f^+_i) = \frac{1}{2} \text{tr} \left( \Psi^0_i \Psi^0_i \left( \sigma^k \right)^T \right) \) \]. Here \( \left( \sigma^k \right)^T \) denotes the transpose of the Pauli matrices for \( k = 1, 2, 3 \).

Realizing \( h_i = g_i h^0_i \) and \( \Psi_i = \left( f^+_i f^+_i f^-if^-i \right) = \left( f^+_i f^+_i f^-if^-i \right) \), and using Eq.(B3), the SU(2) symmetric Heisenberg interaction term is given by

\[ H_j^{SU(2)} = \frac{1}{4} \sum_{<ij>} \left( 1 + h^+_i h^-_j \right) \left( 1 + h^+_j h^-_i \right) \left[ \frac{1}{4} \left( \text{tr} \Psi^0_i \Psi_j \left( \sigma^k \right)^T \right) \left( \text{tr} \Psi^0_j \Psi_j \left( \sigma^k \right)^T \right) \left( f^+_i f^+_i f^+_i f^+_i \right) \right] \]

\[ = -\frac{1}{2} (h^+_i h^-_j + h^+_j h^-_i) (f^+_j f^-if^-i - f'^-_i f'^-_i)(f^-if^-i - f'^-_if'^-_i) \]  

Taking decomposition of the Heisenberg interaction term above into terms involving charge and spin fluctuations separately, uncorrelated mean field contributions and correlated fluctuations, i.e., correlations between charge and spin fluctuations as in the U(1) case, the SU(2) action is rewriten,

\[ S[b_{ia}, f_{ia}, \lambda_i] = \int_0^\beta d\tau \left[ \sum_{i,a=1,2} \left( h^+_i \partial_\tau b_{ia} + f^+_i \partial_\tau f_{ia} \right) + H_j^{SU(2)} \right] \]  

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where
\[ H^{SU(2)}_{i,j} = -\frac{t}{2} \sum_{\langle i,j \rangle} \left[ (f^+_i f^j_{\alpha}) (b^+_j b^1_1 b^1_2 + b^2_1 b^2_2) + c.c. \right. \\
+ (f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta}) (b^+_1 b^1_2 + b^2_1 b^2_2) + c.c. \left. \right] \\
- \frac{t}{2} \sum_{\langle i,j \rangle} \left[ \left( f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta} \right) \left( f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta} \right) (f^1_j f^2_1 - f^2_j f^1_1) \right] (1 + h^1_1 h^1_1) (1 + h^1_1 h^1_1) \\
+ \left( 1 + h^1_1 h^1_1 \right) (1 + h^1_1 h^1_1) \left( f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta} \right) (f^1_j f^2_1 - f^2_j f^1_1) \\
- \left( 1 + h^1_1 h^1_1 \right) \left( 1 + h^1_1 h^1_1 \right) \left( \left( f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta} \right) (f^1_j f^2_1 - f^2_j f^1_1) \right) \left( f^1_2 f^1_{\alpha} - f^1_3 f^2_{\beta} \right) (f^1_j f^2_1 - f^2_j f^1_1) \\
- \mu \sum_{\alpha} \left( 1 - b^1_\alpha \right) \\
- \sum_{\alpha} \left( i\lambda^{(1)} (f^1_1 f^1_{\alpha} + b^1_1 b^1_2) + i\lambda^{(2)} (f^2_1 f^2_{\alpha} + b^1_2 b^1_1) \right. \\
+ i\lambda^{(3)} (f^1_1 f^1_{\alpha} - f^2_1 f^2_{\alpha} + b^1_1 b^1_2 - b^1_2 b^1_1) \right). \] (B6)

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