Mean-Field Description of Phase String Effect in the \( t - J \) Model

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A mean-field treatment of the phase string effect in the \( t - J \) model is presented. Such a theory is able to unite the antiferromagnetic (AF) phase at half-filling and metallic phase at finite doping within a single theoretical framework. We find that the low-temperature occurrence of the AF long range ordering (AFLRO) at half-filling and superconducting condensation in metallic phase are all due to Bose condensations of spinons and holons, respectively, on the top of a spin background described by bosonic resonating-valence-bond (RVB) pairing. The fact that both spinon and holon here are bosonic objects, as the result of the phase string effect, represents a crucial difference from the conventional slave-boson and slave-fermion approaches. This theory also allows an underdoped metallic regime where the Bose condensation of spinons can still exist. Even though the AFLRO is gone here, such a regime corresponds to a microscopic charge inhomogeneity with short-ranged spin ordering. We discuss some characteristic experimental consequences for those different metallic regimes. A perspective on broader issues based on the phase string theory is also discussed.

I. INTRODUCTION

The \( t - J \) Hamiltonian is one of the simplest nontrivial model to describe how doped holes move on the AF spin background and is widely used to characterize the physics in the \( CuO_2 \) layers of cuprates. A tremendous effort has been contributed to the investigation of the \( t - J \) model. The most popular approaches to the metallic phase are often based on the so-called slave-boson method \[1\] in which the degrees of freedom associated with spins are described in terms of fermionic description. There have been many proposals of mean-field ground states based on such a fermionic description of spins, ranging from the earlier fermionic RVB states, \[2\] gauge-theory description, \[3\] SU(2) formalism, \[4\] to possible fractional-statistics. \[5\] However, there is an inherent problem quite general to the fermionic description of spins: approaches based on it usually fail in faithfully producing correct AF correlations especially at small doping.

At half-filling, for example, the exact ground state is known to satisfy the Marshall sign rule \[3\] (for a bipartite lattice) but a fermionic description of spins would show redundant signs: even exchanging two same spins will give rise to a sign change of wavefunction due to the fermionic statistics. Under strict enforcement of no double occupancy constraint, those unphysical signs would not have any effect. But in mean-field approximations, this “sign problem” will always show up and cause serious problem like overall underestimate of AF correlations.

By contrast, the Marshall sign can be easily incorporated into a bosonic description of spin degrees of freedom, where no extra sign problem would be caused by the statistics of bosons. It is the reason contributing to the success of the bosonic RVB description \[4,5\] and its mean-field version – the Schwinger-boson mean-field approach \[1\] in describing spin properties at half-filling. A variational wavefunction based on the bosonic RVB picture can produce \[6,7\] an unrivaled accurate ground-state energy \((-0.3344J\) per bond as compared to the exact numerical value of \(-0.3346J\) per bond for the Heisenberg model), and a generalized description \[8\] can precisely provide not only the ground-state energy, staggered magnetization, but also spin excitation spectrum in the whole Brillouin zone.

A perspective on broader issues based on the phase string theory is also discussed.
motion of doped holes in the AF background. It has been found that spin-mismatches caused by the hopping of doped holes cannot be completely “repaired” through spin flips at low energy. Such a residual nonrepairable effect can be expressed by a path-dependent phase product known as phase string. Due to the phase string effect, a hole slowly moves through a closed path will acquire a nontrivial Berry’s phase. As this phase string effect is very singular locally at a lattice constant scale, its topological effect can be easily lost if a conventional mean-field average is involved — a reason causing the aforementioned spiral instability.

In order to handle such a singular phase string effect hidden in the conventional Schwinger-boson-slave-fermion scheme, a unitary transformation has been introduced to regulate the Hamiltonian such that the local singularity of the phase string (at the scale of one lattice constant) is “gauged away”, while its large distance topological consequence is explicitly incorporated into the Hamiltonian. The resulting exact reformulation of the $t-J$ model is believed to be more suitable for a perturbative treatment, in contrast to the original slave-fermion formalism. The underlying physical implication is that the “holon” and “spinon” defined in the slave-fermion scheme may not be really separable due to the hidden phase string effect, but those in the new formalism may become truly elementary excitations. In the one-dimensional (1D) case, correct Luttinger-liquid behaviors indeed can be reproduced after a mean-field decoupling of the spin and charge degrees of freedom in this new scheme.

In this paper, we develop a generalized mean-field-type theory based on this new formalism of the $t-J$ model in the two-dimensional (2D) case. This theory recovers the well-known Schwinger-boson mean-field state at half-filling while predicts a metallic phase at finite doping without encountering any spiral instability. It offers a unified phase diagram for the $t-J$ model at small doping, in which an insulating AFLRO phase, an underdoped metallic phase with the phenomena of pseudo-gap and charge inhomogeneity, as well as a uniform metallic phase with “optimized” superconducting transition temperature, are all natural consequences happening on a single spin background controlled by bosonic RVB order pairing. The phase string effect plays a crucial role here to connect those different phases together within a single theoretical framework. A short version of this work was published earlier.

**II. MEAN-FIELD THEORY BASED ON PHASE STRING EFFECT**

In the standard slave-fermion formalism of the $t-J$ Hamiltonian, electron annihilation operator $c_{i\sigma}$ is written as

$$c_{i\sigma} = f_i^\dagger b_{i\sigma} (-\sigma)^i,$$  \hspace{1cm} (2.1)

in which $f_i^\dagger$ is fermionic “holon” creation operator and $b_{i\sigma}$ is bosonic (Schwinger-boson) “spinon” annihilation operator, satisfying no double occupancy constraint

$$f_i^\dagger f_i + \sum_\sigma b_{i\sigma}^\dagger b_{i\sigma} = 1.$$ \hspace{1cm} (2.2)

The $t-J$ model, $H_{t-J} = H_t + H_J$, is composed of two terms: the hopping term $H_t$ is given by

$$H_t = -t \sum_{\langle ij \rangle, \sigma} (\sigma) f_i^\dagger f_j b_{j\sigma}^\dagger b_{i\sigma} + H.c.,$$ \hspace{1cm} (2.3)

and the superexchange term is

$$H_J = -\frac{J}{2} \sum_{\langle ij \rangle, \sigma\sigma'} b_{i\sigma}^\dagger b_{j\sigma'}^\dagger b_{j\sigma} b_{i\sigma'}.$$ \hspace{1cm} (2.4)

Note that the staggered phase factor $(-\sigma)^i$ in (2.1) is introduced to explicitly track the Marshall sign, which leads to the negative sign in (2.4). A sign $\sigma = \pm 1$ then appears in the hopping term (2.3) which is the origin of the phase string effect mentioned in the Introduction. Due to such a sign, a hole moving from a site $a$ to an another site $b$ will acquire a sequence of signs, i.e., a phase string as shown in Fig. 1, which has been shown to be nonrepairable by the spin flip process governed by $H_J$. It implies that the slave-fermion formalism of the $t-J$ model cannot be treated in a perturbative way in doped case.
A. Phase string representation

It has been shown that the above singular effect of phase string can be regulated after a unitary transformation. The resulting new formalism is known as the phase string representation. The hopping term $H_t$ in this new representation becomes

$$H_t = -t \sum_{(ij)\sigma} \left( e^{iA_{ij}^s} \right) h_i^\dagger h_j \left( e^{i\sigma A_{ji}^h} \right) b_i^\dagger b_{i\sigma} + H.c. \quad (2.5)$$

and the superexchange term $H_J$ reads

$$H_J = -\frac{J}{2} \sum_{(ij)\sigma\sigma'} \left( e^{i\sigma A_{ij}^s} \right) b_i^\dagger b_{j\sigma} \left( e^{i\sigma' A_{ji}^h} \right) b_{j\sigma'} b_{i\sigma'}. \quad (2.6)$$

Note that the fermionic operator $f_i$ now is replaced by a bosonic holon operator $h_i$ in this new formalism. So one role of the phase string effect is to turn holons from fermions into bosons. Both holon and spinon are now described by bosonic operators which still satisfy the following no double occupancy constraint

$$h_i^\dagger h_i + \sum_{\sigma} b_i^\dagger b_i = 1. \quad (2.7)$$

In this new formalism, the singular phase string effect, as represented by the sign $\sigma$ in the hopping term (2.3) of the original slave-fermion representation, is "gauged away", but its topological effect is left and exactly tracked by lattice gauge fields $A_{ij}^s$ and $A_{ij}^h$. These fields are defined as follows

$$A_{ij}^f \equiv A_{ij}^s - \phi_{ij}^0 \quad (2.8)$$

with

$$A_{ij}^s = \frac{1}{2} \sum_{l \neq i,j} [\theta_i(l) - \theta_j(l)] \left( \sum_{\sigma} \sigma n_{l\sigma}^b \right), \quad (2.9)$$

$$\phi_{ij}^0 = \frac{1}{2} \sum_{l \neq i,j} [\theta_i(l) - \theta_j(l)], \quad (2.10)$$

and

$$A_{ij}^h = \frac{1}{2} \sum_{l \neq i,j} [\theta_i(l) - \theta_j(l)] n_{l}^h. \quad (2.11)$$

Here $n_{l\sigma}^b$ and $n_{l}^h$ are spinon and holon number operators, respectively. $\theta_i(l)$ is defined as an angle

$$\theta_i(l) = \text{Im} \ln (z_i - z_l) \quad (2.12)$$

with $z_i = x_i + iy_i$ representing the complex coordinate of a lattice site $i$.

The physical meaning of $A_{ij}^s$ and $A_{ij}^h$ have been discussed in Ref. [17]: $A_{ij}^s$ and $A_{ij}^h$ describe quantized flux tubes bound to spinons and holons, respectively (Fig. 2 illustrates the case for $A_{ij}^h$). Furthermore, the field $\phi_{ij}^0$ describes a uniform flux threading through the 2D plane with a strength $\pi$ per plaquette: $\sum_\partial \phi_{ij}^0 = \pm \pi$. It is also noted that a $\pi$-flux neutral topological excitation has been previously discussed in the pure Heisenberg model, which resembles a quantized flux line in the mixed phase of a BCS superconductor. Here the flux quanta are bound to the doped holes due to the phase string effect.

Electron operator in this representation becomes

$$c_{i\sigma} = h_i^\dagger b_{i\sigma} (-\sigma)^{i} e^{i\Theta_{i\sigma}^{string}}. \quad (2.13)$$

Here the nonlocal phase factor $e^{i\Theta_{i\sigma}^{string}}$ precisely keeps the track of the singular part of the phase string effect and is defined by
\[ \Theta^{string}_{i\sigma} = \frac{1}{2} [\Phi_i^b - \sigma \Phi_i^h], \]  
with

\[ \Phi_i^b = \sum_{l \neq i} \theta_i(l) \left( \sum_{\alpha} \alpha n_i^b l_{\alpha} - 1 \right), \]  
and

\[ \Phi_i^h = \sum_{l \neq i} \theta_i(l) n_i^h. \]

**B. Mean-field approximation**

For the sake of clarity, in the following we first consider the superexchange term \( H_J \) and then include the hopping term \( H_t \), due to different natures represented by them.

1. Generalized mean-field treatment of \( H_J \)

At half-filling, the mean-field theory based on the bosonic RVB picture is known as the Schwinger-boson mean-field theory which was first introduced by Arovas and Auerbach [11]. Such a mean-field is characterized by a bosonic RVB order parameter

\[ \Delta^s = \sum_{ij} \langle b_{i\sigma} b_{j-\sigma} \rangle \]  
for the nearest-neighbor sites \( i \) and \( j \) \([i = nn(j)]\).

The present formalism only differs from the Schwinger-boson, slave-fermion formalism in doped case, where a gauge field \( A_{ij}^h \) emerges. Since spinons are subject to this gauge-field \( A_{ij}^h \) in \( H_J \), it is natural to incorporating the link variable \( e^{-i\sigma A_{ij}^h} \) into the order parameter \( 2.17 \). Namely,

\[ \Delta_{ij}^s = \sum_{\sigma} \langle e^{-i\sigma A_{ij}^h} b_{i\sigma} b_{j-\sigma} \rangle. \]

\( \Delta_{ij}^s \) defined here is then “gauge-invariant” under an “internal” gauge transformation: \( A_{ij}^h \rightarrow A_{ij}^h + \theta_i - \theta_j \), and \( b_{i\sigma} \rightarrow b_{i\sigma} e^{i\sigma \theta_i} \).

Based on such an order parameter, one may write down the mean-field version of \( H_J \) in \( 2.6 \) in a standard procedure

\[ H_J^s = -\frac{J}{2} \sum_{(ij)\sigma} (\Delta_{ij}^s)^2 e^{-i\sigma A_{ij}^h} b_{i\sigma} b_{j-\sigma} - H.c. + \frac{J}{2} \sum_{(ij)} |\Delta_{ij}^s|^2 + \lambda \left( \sum_{i\sigma} b_{i\sigma} b_{i\sigma} - (1 - \delta)N \right), \]

where the last term with a Lagrangian multiplier \( \lambda \) is introduced to enforce the condition of total spinon number, with \( N \) denoting the total lattice number and \( \delta \) doping concentration. In order to diagonalize \( H_J^s \), we introduce the following Bogoliubov transformation

\[ b_{i\sigma} = \sum_m \left( u_{m\sigma}(i) \gamma_{m\sigma} - v_{m\sigma}(i) \gamma_{m-\sigma}^\dagger \right), \]

and seek the solution

\[ [H_J^s, \gamma_{m\sigma}^\dagger] = E_m \gamma_{m\sigma}^\dagger, \]  
\[ [H_J^s, \gamma_{m\sigma}] = -E_m \gamma_{m\sigma}. \]
Here $\gamma_{m\sigma}$ and $\gamma_{m\sigma}^\dagger$ are bosonic annihilation and creation operators, respectively, for an eigenstate with quantum number $m$ and spin $\sigma$. In terms of bosonic commutation relations, one easily finds that $u_{m\sigma}(i)$ and $v_{m\sigma}(i)$ satisfy

$$\sum_m [u_{m\sigma}(i)u_{m\sigma}^*(j) - v_{m\sigma}(i)v_{m\sigma}^*(j)] = \delta_{ij}, \quad (2.23)$$

and

$$\sum_m [u_{m\sigma}(i)v_{m-\sigma}(j) - v_{m\sigma}(i)u_{m-\sigma}(j)] = 0. \quad (2.24)$$

According to (2.19), we have

$$[H_s', b_{n\sigma}] = \frac{J}{2} \sum_{j = nn(i)} \Delta_{ij} e^{-i\sigma A_{ji}} b_{j-\sigma}^\dagger - \lambda b_{n\sigma}. \quad (2.25)$$

Then by using (2.20), (2.21) and (2.22), it is straightforward to derive the following relations from (2.25):

$$- E_m u_{m\sigma}(i) = - \frac{J}{2} \sum_{j = nn(i)} \Delta_{ij} e^{-i\sigma A_{ji}} v_{m-\sigma}^*(j) - \lambda u_{m\sigma}(i), \quad (2.26)$$

$$- E_m v_{m\sigma}(i) = \frac{J}{2} \sum_{j = nn(i)} \Delta_{ij} e^{-i\sigma A_{ji}} u_{m-\sigma}^*(j) + \lambda v_{m\sigma}(i). \quad (2.27)$$

We can further express $u_{m\sigma}(i)$ and $v_{m\sigma}(i)$ by the “one-particle” wavefunction $w_{m\sigma}(i)$ as follows

$$u_{m\sigma}(i) = u_m w_{m\sigma}(i), \quad (2.28)$$

$$v_{m\sigma}(i) = v_m w_{m\sigma}(i), \quad (2.29)$$

where $u_m$ and $v_m$ will be taken to be real and satisfy

$$u_m^2 - v_m^2 = 1. \quad (2.30)$$

Then $w_{m\sigma}(i)$ is normalized following from (2.30):

$$\sum_m w_{m\sigma}(i)w_{m\sigma}^*(j) = \delta_{ij}. \quad (2.31)$$

Equations (2.26) and (2.27) then reduce to an eigen-equation for the one-particle wavefunction $w_{m\sigma}(i)$:

$$\xi_m w_{m\sigma}(i) = - \frac{J}{2} \sum_{j = nn(i)} \Delta_{ij} e^{-i\sigma A_{ji}} w_{m-\sigma}^*(j). \quad (2.32)$$

The eigenvalue $\xi_m$ in (2.32) is related to $E_m$ and $u_m$ and $v_m$ as follows

$$\xi_m = -(E_m - \lambda_m)\frac{u_m}{v_m} = (E_m + \lambda_m)\frac{v_m}{u_m}. \quad (2.33)$$

Here $\lambda_m$ is the same as the Lagrangian multiplier $\lambda$, but we write it in a general form because later it will be modified once the hopping term is introduced. In terms of (2.33) and (2.30), one obtains

$$E_m = \sqrt{\lambda_m^2 - \xi_m^2}, \quad (2.34)$$

and

$$|u_m| = \frac{1}{\sqrt{2}} \left( \frac{\lambda_m}{E_m} + 1 \right)^{1/2}, \quad (2.35)$$

$$|v_m| = \frac{1}{\sqrt{2}} \left( \frac{\lambda_m}{E_m} - 1 \right)^{1/2}. \quad (2.36)$$
The signs of $u_m$ and $v_m$ are determined up to $sgn(v_m/u_m) = sgn(\xi_m)$. As a convention we will always choose $u_m = |u_m|$ and $v_m = |v_m|sgn(\xi_m)$.

Thus $H^\xi$ is diagonalized as $H^\xi = \sum_{m,\sigma} E_m \gamma^\dagger_{m\sigma} \gamma_{m\sigma} + \text{const.}$ according to (2.21) and (2.22). The order parameter $\Delta_{ij}$ can be self-consistently determined by the definition (2.18) as

$$\Delta^s_{ij} = \sum_{m,\sigma} e^{-i\sigma A^h_{ij}} w_{m\sigma}(i) w_{m,-\sigma}(j) (-u_m v_m) \left[ 1 + \sum_\alpha (\gamma^\dagger_{i\alpha} \gamma_{m\alpha}) \right].$$

(2.37)

In the following we will always consider the solution of a real order parameter $\Delta^s_{ij}$. In this case, it can be checked self-consistently that $w_{m\sigma} = w^*_{m,-\sigma}$ according to (2.32) and $(\Delta^s_{ij})^* = \Delta^s_{ij}$ in terms of (2.37). The order-parameter equation may be further simplified if one multiplies (2.37) by $(\Delta^s_{ij})^*$ and sums over $(ij)$ with using (2.32):

$$\sum_{\langle ij \rangle} |\Delta^s_{ij}|^2 = \sum_m \frac{\xi^2_m}{\beta E_m} \coth \frac{\beta E_m}{2},$$

(2.38)

with $\langle \gamma^\dagger_{i\alpha} \gamma_{m\alpha} \rangle = 1/(e^{\beta E_m} - 1)$ and $\beta \equiv 1/k_BT$. Finally, the condition

$$\left\langle \sum_{i\sigma} b^\dagger_{i\sigma} b_{i\sigma} \right\rangle = (1 - \delta)N,$$

(2.39)

which is enforced by the Lagrangian multiplier in (2.19) and can be rewritten as

$$2 - \delta = \frac{1}{N} \sum_{m \neq 0} \lambda_m E_m \coth \frac{\beta E_m}{2} + n^b_{BC},$$

(2.40)

where $n^b_{BC}$ is introduced to describe the contribution from $E_m = 0$ state (denoted by $m = 0$) when the Bose condensation of spinons occurs. [20] In comparison with the zero-doping Schwinger-boson mean-field theory, the above Bogoliubov-de Gennes scheme at finite doping mainly differs in the one-particle eigenequation (2.32) (and the resulting energy spectrum $\xi_m$ and wavefunction $w_{m\sigma}(i)$). One may simply recover the Schwinger-boson mean-field results by setting $A^h_{ij} = 0$ in (2.32) and obtaining $\xi_k = -J \Delta^s_0 (\cos k_x a + \cos k_y a)$ and the Bloch wavefunction $w_{k\sigma} = \frac{1}{\sqrt{N}} e^{i\sigma k \cdot r}$ in the no-hole case.

So the doping effect has entered the above mean-field theory in two ways: one is through the particle number condition in (2.39); the other is through the gauge field $A^h_{ij}$. For the mean-field theory to work, $A^h_{ij}$ has been implicitly assumed as a time-independent field. But with holons moving around, $A^h_{ij}$ will usually gain a dynamic effect. To see this, let us consider the following gauge-invariant quantity

$$\sum_C A^h_{ij} = \pi \sum_{l \in C} n^h_l,$$

(2.41)

where $C$ is an arbitrary counter-clockwise closed path. If one redefines

$$n^h_l = \delta + \delta n^h_l,$$

(2.42)

with $\delta n^h_l = n^h_l - \delta$, then correspondingly

$$A^h_{ij} = \tilde{A}^h_{ij} + \delta A^h_{ij},$$

(2.43)

where

$$\sum_C \tilde{A}^h_{ij} = \pi \delta S_C \frac{a}{a^2} \equiv \delta \frac{S_C}{a^2},$$

(2.44)

($S_C$ denotes the area of a loop $C$ and $a$ is the lattice constant) and

$$\sum_C \delta A^h_{ij} = \pi \sum_{l \in C} \delta n^h_l.$$

(2.45)
So the dynamics of $A_{ij}^h$ is determined by the fluctuations of the density of holons on lattice. But since spinons and holons here are treated as independent degrees of freedom, one may neglect the dynamical effect of $\delta A_{ij}^h$ on spinon part at the mean-field level and replace it by some random flux fluctuation $s$ with a strength per plaquette equal to $\delta \phi$ (One may estimate $\delta \phi \approx \pi \sqrt{\langle \delta n^2 \rangle}$). This can be justified at low temperature when a Bose condensation of holons (which corresponds to a superconducting condensation as shown later) occurs, where $\delta A_{ij}^h$ is expected to be substantially suppressed. On the other hand, however, in the high temperature phase where the motion of holons is much less coherent, the fluctuation effect of $\delta A_{ij}^h$ can dominate over $A_{ij}^h$ and the separation of the latter from $\bar{A}_{ij}^h$ then becomes meaningless. In this case, one may approximately describe the effect of $A_{ij}^h$ as a collection of randomly distributed $\pi$ flux quanta with the number equal to that of holons. In both limits, the dynamics of $A_{ij}^h$ may be neglected.

2. Including the hopping term $H_t$

First of all, we note that the wavefunction $w_{m\sigma}(i)$ as the solution of the linear equation (2.32) is not unique, and it can be always multiplied by an arbitrary global phase factor $e^{i\sigma \chi_m}$: i.e.,

$$w_{m\sigma}(i) \rightarrow e^{i\sigma \chi_m}w_{m\sigma}(i),$$

(2.46)

without changing the order parameter $\Delta_{ij}^s$ and the mean-field state. Correspondingly the Bogoliubov transformation can be generally rewritten as

$$b_{i\sigma} = \sum_m \left( u_m \gamma_{m\sigma} - v_m \gamma_{m-\sigma} \right) e^{i\sigma \chi_m} w_{m\sigma}(i).$$

(2.47)

In particular, $e^{i\sigma \chi_m}$ can depend on the holon configurations because the Hilbert space of $b_{i\sigma}$ is only well-defined at each given holon configuration due to the no-double-occupancy constraint. The hopping term will mix the Hilbert space of $b_{i\sigma}$ at different holon configurations, and such a freedom in phase choice can be fixed by optimizing the hopping integral of holons below.

Now consider the hopping term $H_t$ in (2.5). By using the Bogoliubov expression for spinon operators, a straightforward calculation gives

$$\left< \sum_{\sigma} e^{i\sigma A_{ji}^h b_{j\sigma}^\dagger b_{i\sigma}} \right> = \sum_{m\sigma} e^{i\sigma A_{ji}^h w_{m\sigma}^*(j) w_{m\sigma}(i)} e^{-i\sigma \Delta \chi_m} \left[ v_m^2 + (u_m^2 + v_m^2) \langle \gamma_{m\sigma} \gamma_{m-\sigma} \rangle \right].$$

(2.48)

Note that $\Delta \chi_m$ in the above expression denotes the difference of $\chi_m$ before and after the holon changes the position. If one simply chooses $\Delta \chi_m = 0$, namely, the phases of $w_{m\sigma}(i)$ to be the same for all hole configurations, then the right-hand side of (2.48) vanishes for the nearest-neighboring $i$ and $j$. This can be verified by noting that $w_{m\sigma}(i) \equiv (-1)^i w_{m\sigma}$ is also a solution of (2.32) with an eigenvalue $\xi_m = -\xi_m$ and the cancellation in (2.48) stems from the fact that those quantities like $u_m^2$ and $v_m^2$ only depend on $E_m$ in (2.48) which is symmetric under $\xi_m \rightarrow -\xi_m$. But such a cancellation is removable by a simple choice of the phase shift in $e^{i\sigma \chi_m}$ at different holon configurations when each time a holon changes sublattice sites:

$$e^{i\sigma \chi_m} \rightarrow [-sgn(\xi_m)] \times e^{i\sigma \chi_m},$$

(2.49)

$$e^{-i\sigma \Delta \chi_m} = -sgn(\xi_m).$$

(2.50)

Then, one finds

$$B_0 = \frac{1}{2N} \sum_{(ij)\sigma} \left< e^{i\sigma A_{ji}^h b_{j\sigma}^\dagger b_{i\sigma}} \right> = \frac{1}{2N} \sum_{m\sigma} B_m^0 \left[ v_m^2 + (u_m^2 + v_m^2) \langle \gamma_{m\sigma} \gamma_{m-\sigma} \rangle \right],$$

(2.51)

where $B_m^0 \equiv \sum_{(ij)} e^{i\sigma A_{ji}^h w_{m\sigma}^*(j) w_{m\sigma}(i)} [-sgn(\xi_m)]$ is given by

$$B_m^0 = -sgn(\xi_m) \sum_{(ij)} e^{i\sigma A_{ji}^h w_{m\sigma}^*(j) w_{m\sigma}(i)}$$

$$= sgn(\xi_m) \frac{\xi_m}{2J_z} \sum_i w_{m\sigma}^*(i) w_{m\sigma}(i)$$

$$= \frac{\xi_m}{2J_z} > 0. $$

(2.52)
In obtaining the second line above, we have used (2.32) with \( \Delta_{ij}^s = \Delta^s \) and \( J_s \equiv \frac{1}{2} \Delta^s J \).

Holons thus acquire a finite hopping integral without introducing any extra order parameter. The effective holon Hamiltonian is given by:

\[
H_h = -t_h \sum_{\langle ij \rangle} e^{iA_{ij}^h} s_{ij}^h + H.c.,
\]

(2.53)

which is derived from \( H_t \) with an effective hopping integral

\[
t_h \equiv tB_0.
\]

(2.54)

It is important to note that such a finite kinetic energy \( (t_h \sim t) \) that each holon has gained on the present mean-field spin background cannot be similarly realized in the slave-fermion-Schwinger-boson scheme, exactly due to the hidden phase-string effect: the sign \( \sigma = \pm 1 \) in \( (2.32) \) will always lead to \( t_h = 0 \) and make a spiral twist (a new order parameter in favor of hole hopping) necessary in any local mean-field treatment.

Finally, to be consistent, the hopping effect on the spinon part is solely represented by a shift from \( \lambda_m \) to \( \lambda_m^0 \) in (2.61). The Bogoliubov transformation (2.61) remains unchanged and so do \( u_m \) and \( \bar{v}_m \) defined in (2.35) and (2.36), so long as the renormalized \( \lambda_m \) is used. The Lagrangian multiplier \( \lambda \) in (2.61) is still determined by (2.40) where both \( \lambda_m \) and \( E_m \) should be replaced by the renormalized ones in (2.61) and (2.61). Finally, the self-consistent equation (2.38) for the RVB pairing order parameter maybe rewritten as

\[
\lambda_m = \lambda - \frac{J_h}{J_s} |\xi_m|.
\]

(2.61)
\[ \Delta^* = \frac{1 - 2\delta}{4N} \sum_m \frac{\xi_m^2}{J_m E_m} \coth \frac{\beta E_m}{2}. \]  

(Note that if the Bose condensation occurs, one may separate the contribution from the condensation part on the right-hand-side by \( \Delta_{BC}^* \equiv (1 - 2\delta)\xi_0^2 n_{BC}^b / 4J_s \lambda_0 \). In obtaining (2.62), we have used an approximate relation \( 1/(2N) \sum_{(ij)} \langle (\Delta_0)_{ij} \rangle_h \approx \Delta^2/(1 - 2\delta) \) at \( \delta < 0.5 \) limit. Such a relation can be obtained by assuming \( \Delta_0^* = \Delta_1^* \) when \( i \) and \( j \) belongs to occupied sites and \( \Delta_0^* = 0 \) if \( i \) or \( j \) is at hole site and by noting that each hole accounts for \( \Delta_{ij}^* = 0 \) at four adjacent bonds at dilute-hole limit which leads to \( \Delta^* = (1 - 2\delta)\Delta_1^* \).

III. PHASE DIAGRAM

A. Unified bosonic RVB phase

Our mean-field theory has been constructed based on a single bosonic RVB order parameter \( \Delta^* \). Such an order parameter controls short-range spin-spin correlations in both undoped and doped regime. Fig. 3 shows a typical region of \( \Delta^* \neq 0 \) obtained by solving the mean-field equations which has been briefly discussed in Ref. [13]. It obviously covers the whole experimentally interested temperature (from \( T = 0 \) to \( T \sim 0.5 - 0.9 J_B \)) and doping (from \( \delta = 0 \) to \( \delta > 0.3 \)) regime. Several low-temperature regions within this phase as marked in Fig. 3, including the superconducting phase, will be discussed in the following sections. The normal-state within this phase will correspond to a “strange metal” phase, where magnetic and transport properties are expected to be different from conventional metals. It is noted that in the bosonic RVB description of spin degrees of freedom, the order parameter \( \Delta^* \) does not directly correspond to an energy gap, in contrast to the fermionic RVB theory (the latter is similar to the BCS theory in mathematical structure). Also note that the crossover from \( \Delta^* \neq 0 \) phase to \( \Delta^* = 0 \) phase at high temperature is similar to the half-filling case [11] which does not correspond to a real phase transition.

In obtaining \( \Delta^* \) in Fig. 3 by solving (2.62), one also needs to determine the spectrum \( \xi_m \) from (2.32) and decide the chemical potential \( \lambda \) in terms of (2.40). We have chosen the parameter \( J_h = \delta J \) (which corresponds to \( t \sim J \)) and solved \( \xi_m \) under \( A_{ij}^b = \tilde{A}_{ij}^b \), but other choices of \( J_h \) as well as including the fluctuating part \( \delta \tilde{A}_{ij}^b \) do not change significantly the range covered by \( \Delta^* \neq 0 \). The effect of \( \delta \tilde{A}_{ij}^b \) will be the subject of discussion in the next section, and we will always use the same \( J_h \) below.

Although \( \Delta^* \neq 0 \) practically covers the whole doping regime, at a larger doping concentration, this mean-field theory may no longer be energetically favorable due to the competition between the hopping and superexchange energies. Actually, the phase string effect itself is an indication that the bosonic description of spins leads to frustration of the motion of doped holes, and vice versa. With the increase of doping concentration, one possibility is that eventually a statistical-transmutation may occur to effectively turn bosonic spinons into fermionic ones as to be discussed in Sec. IV. Beyond such a point, the present mean-field theory will break down, which may determine a crossover to the so-called overdoped regime. We will explore this issue elsewhere.

B. Bose condensation of spinons: AF ordering vs. phase separation

1. AFLRO and insulation phase

At half-filling, the spinon spectrum \( E_m \) is known to be gapless at zero doping and zero temperature which ensures a Bose condensation [20] of spinons. Such a Bose condensation of spinons, as represented by \( n_{BC}^b \neq 0 \) in (2.40), describes a long-range AF spin ordering. [21] The Bose condensation or long-range AF order can be sustained up to a finite temperature \( T_N > 0 \) if the three-dimensional effect (interlayer coupling) is included. In the following, we consider how this AFLRO picture evolves at finite doping.

Based on the expression (2.13), spin operators, \( S_i^z \) and \( S_{\pm i} \), can be easily written down in terms of spinon operator \( b_{\sigma} \) after using the constraint (2.7):

\[ S_i^z = \frac{1}{2} \sum_\sigma \sigma \langle \delta b_{\sigma}^\dagger b_{\sigma} \rangle, \]  

(3.1)
\[ S_i^+ = b_i^\dagger b_i (-1)^i e^{i \phi_i} \]

and \( S_i^- = (S_i^+)^\dagger \).

At \( \delta = 0 \), one has \( \Phi_i^h = 0 \), and the Bose condensation leads to

\[ \langle S_i^+ \rangle \propto (-1)^i, \]

i.e., an AFLRO. But at \( \delta \neq 0 \), even when the spinons are Bose-condensed, \( \langle S_i^+ \rangle \) should generally vanish due to the fact that

\[ \langle e^{i \phi_i^h} \rangle = 0. \]

The proof here is straightforward. Note that in the definition of \( \Phi_i^h \) in \( (2.16) \), the angle \( \theta_i(l) \) \([2.12]\) can be transformed as

\[ \theta_i(l) \rightarrow \theta_i(l) + \phi \]

for an arbitrary \( \phi \) without changing \( A_{ij}^h \), \( A_{ij}^f \), and thus the Hamiltonian. But \( e^{i \phi_i^h} \) \([2.16]\) changes accordingly

\[ e^{i \phi_i^h} \rightarrow e^{i \phi_i^h} \times e^{i \phi N^h}, \]

Here \( N^h \) is the total holon number. Thus the average of such a phase must vanish at finite doping as given in \([1.4]\). Since \( \Phi_i^h \) describes vortices centered at holons, it is like a free-vortex phase as holons move around freely in metallic phase, which resembles a disordered phase in a Kosterlitz-Thouless-type transition.

Only in the case that holons are localized (i.e., in insulating phase) such that the phase string effect is ineffective, the AFLRO may be recovered. In this insulating phase, holons are perceived by spinons as localized vortices like in the mixed state of a type-II superconductor, and by forming “supercurrents” to screen those vortices, \( \Phi_i^h \) in \( S_i^+ \) can be effectively canceled out by the opposite vorticities generated from spinons. After all, the phase string effect is no longer important if the motion of holons is limited. We do not know if the localization of holons can happens intrinsically or has to be under some external factors like impurity effect. But we expect such an insulating phase to exist only at a very dilute density of holons at the expense of latter’s kinetic energy.

2. Bose condensation of spinons in metallic phase: underdoping

We have shown that the AFLRO must be absent in metallic phase. One may naturally wonder if the Bose condensation of spinons can still persist into metallic phase, and if it does, then what is its physical meaning?

To answer these questions, let us first to inspect how the spinon spectrum \( E_m \) is modified by doping. In Fig. 4, we compare the spinon density of states \( \rho_s(E) \) at \( \delta = 1/7 \approx 0.143 \) (solid curve) with the \( \delta = 0 \) case (diamond curve in the insert). Here \( \rho_s(E) \) is defined by

\[ \rho_s(E) = \frac{1}{N} \sum_m \delta(E - E_m). \]

One notices that a unique peak-structure is clearly exhibited at \( \delta = 0.143 \). This can be easily understood by noting that the spinon spectrum \( E_m \) is basically determined by \( \xi_m \) which, as the solution of \( (2.40) \), has a Hofstadter structure (or the Landau levels in the continuum limit) due to a uniform flux \( (\phi = \pi \delta \) per plaquette) represented by the vector potential \( A_{ij}^f \) threading through the square lattice. The broadening of the solid curve in Fig. 4 is due to the redistribution of eigenstates under the fluctuating flux \( \delta A_{ij}^h \), which is treated as a random flux (in white noise limit) here with a maximum strength chosen at \( \delta \phi = 0.3 \delta \) per plaquette. By contrast, the dashed curve marks the positions of sharp peaks of density of states in the limit of \( \delta \phi = 0 \).

We find that the Bose condensation of spinons can still occur at \( \delta = 0.143 \) with \( \delta \phi = 0.3 \delta \) (but not at \( \delta \phi = 0 \)) as the solution of \( (2.40) \). Recall that the spinon Bose condensation stems from the equation \( (2.40) \) with a nonzero \( n_{BC}^h \) representing the density of spinons staying at \( E_m = 0 \) state. In this case, there would be no solution at low temperature unless \( \lambda \) takes a value to make \( E_m \) gapless such that \( n_{BC}^h \neq 0 \) can balance the difference between the left and right side of the equation, similar to the half-filled case. \([2]\) In particular, such a Bose condensation is found to be sustained up to a finite temperature \( T_{BC} \sim 0.21J \) even in the present 2D case. This is due to the vanishingly
small weight near \( E = 0 \) in the density of states (in Fig. 4, there is a small tail in the solid curve which extends to \( E = 0 \)), where the spinon excitations at low-temperature are not sufficient to destroy the Bose condensation as first pointed out in Ref. [21]. It is noted that in principle the strength \( \delta \phi \) of the random fluctuations of \( \delta A_{ij}^h \) should be self-consistently determined by the density fluctuations of holons. But here for simplicity we just treat \( \delta \phi \) as a parameter and then study the qualitative characteristics under different values of \( \delta \phi \). The actual strength of the fluctuations of \( A_{ij}^h \) will be only crucial in determining the location of the phase boundary.

**Phase separation** Note that the Bose condensation means a thermodynamic number of spinons staying at \( E_m = 0 \) — the lowest energy state which corresponds to the band edges of the spectrum \( \xi_m \). So due to the Bose condensation, such quantum states will acquire a macroscopic meaning. But these band edge states of \( \xi_m \) are very sensitive to the fluctuations of \( A_{ij}^h \) and the density of holons. Physically, the density of holons is fluctuating in real space (which is the reason leading to the fluctuations of \( A_{ij}^h \)) and there always exist those configurations in which the density of holes are relatively dilute in some areas where the flux described by \( A_{ij}^h \) is reduced such that the band edge energies of \( \xi_m \) can be close to \( \pm 2J_s \). Since the probability would be small for such kind of inhomogeneous hole configurations, the density of states generally looks like a tail — i.e., the Lifshitz tail— near the band edges. Hence, the corresponding Bose-condensed state will generally look like having a charge inhomogeneity, or, phase separation, with spinons condensing into hole-deficient regions to form short-range spin ordering. The true AFLRO is absent here.

**Pseudo-gap behavior** The Bose condensation of spinons will also lead to a pseudo-gap phenomenon. In magnetic aspect, for example, the density of states shown in Fig. 4 indicates the suppression of spinon density of states between zero and the lowest peak, which stabilizes the Bose condensation as mentioned earlier. Since in the Bose condensation case there must be some residual density extending to \( E_m = 0 \), a pseudo spin gap is thus present in \( \rho_s(E) \). Its effect in the dynamic spin susceptibility will be discussed later. In the transport aspect, holons which are the charge carriers are scattered off by the gauge field \( A_{ij}^s \) according to the holon effective Hamiltonian (2.53). Anomalies in transport properties have been found in Ref. [21] with interesting experimental features in the similar effective Hamiltonian, where fluctuating fluxes depicted by \( A_{ij}^s \) play a central role. But the Bose condensation of spinons will lead to a substantial suppression of \( A_{ij}^s \) and thus a reduction of scattering to holons. Hence, the Bose condensation also provides an explanation for the so-called pseudo-gap phenomenon shown in the underdoped high-\( T_c \) cuprates, where the transport properties deviate from the high temperature ones below some characteristic temperature scale.

Therefore, if the Bose condensation of spinons happens in metallic phase, it will result in a phase-separation or spin pseudo-gap phase without the AFLRO. With the increase of \( \delta \), the reduction of the left hand side of (2.40) will eventually make the Bose condensation term, if exists, disappear from the right hand side. So the Bose condensation in general may only exist at small doping regime, which can be defined as the “underdoping” regime. In Fig. 3, the shaded curve sketches such a region outside the true AFLRO phase which is in a much narrower region (dotted curve) at finite doping.

**C. Superconductivity**

In the phase-string representation, the operator of superconducting order parameter

\[
\hat{\Delta}_{ij}^{SC} = \sum_\sigma \sigma c_{i\sigma} c_{j,-\sigma}
\]

(3.8)
can be expressed in terms of (2.13) as follows

\[
\hat{\Delta}_{ij}^{SC} = \hat{\Delta}_{ij}^s \left( h_i^e e^{i A^b_{ij}} \right) \left( h_j^e e^{i A^b_{ij}} \right) (-1)^i,
\]

(3.9)
in which

\[
\hat{\Delta}_{ij}^s = \sum_\sigma e^{-i \sigma A^s_{ij}} b_{i\sigma} b_{j,-\sigma}.
\]

(3.10)

This is the basic expression to be used in the following discussion of superconducting condensation.

**1. Mechanism**

For the sake of simplicity, we will focus on the nearest-neighboring pairing with \( i = nn(j) \) below. Since the whole mean-field phase is built on
\[ \langle \hat{\Delta}_i^s \rangle = \Delta^s \neq 0, \] (3.11)

the electron pairing order parameter \( g \Delta_{ij}^{SC} = \langle \hat{\Delta}_{ij}^s \rangle \) can be written as

\[ \Delta_{ij}^{SC} = \Delta^s \left( \left( h_i^\dagger e^{+\Phi_i^b} \right) \left( h_j^\dagger e^{+\Phi_j^b} \right) \right) (-1)^i. \] (3.12)

We see that the spinons are always paired in the present phase, as described by \( \Delta^s \), up to a temperature scale \( \sim J \) at small doping. Thus, in order to have a real superconducting condensation below a transition temperature \( T_c \), the holon part has to undergo a Bose condensation or, strictly speaking in 2D, a superfluid transition in the Kosterlitz-Thouless sense (recall that both spinon and holon are bosonic in the present representation).

One may notice that this superconducting condensation picture is somewhat similar to that in the slave-boson mean-filed theory. \[ \] But there are two crucial differences.

Firstly, the spinon pairing in the present case practically covers the whole superconducting and normal-state regime that we are interested in. In other words, \( \Delta^s \neq 0 \) in the present mean-field theory defines a “strange” metal, and the normal-state anomalies of experimental measurements in the cuprates, including the magnetic properties and the transport properties, are all supposed to happen within such a phase. In contrast, in the slave-boson mean-field approach the fermionic spinon pairing is directly related to the gap in the spinon spectrum and has to disappear at a much lower temperature scale beyond which “strange” metallic properties presumably start to show up.

Secondly, the Kosterlitz-Thouless transition temperature of holons are believed to be much higher than the real \( T_c \) in the cuprates, and thus one has to introduce other mechanism (e.g., gauge-field fluctuations) to bring down the temperature scale in the slave-boson mean-field approximation. On the other hand, there is a unique feature in \( \), namely, the presence of phases like \( e^{\pm \Phi_i^b} \). Here \( \Phi_i^b \) represents a structure of vortices (anti-vortices) centered at \( \uparrow (\downarrow) \) spinons. At \( T = 0 \), all \( \uparrow \) and \( \downarrow \) spinons are paired up at a finite length scale and so are the vortices and anti-vortices in \( \Phi_i^b \), which implies \( \Delta_{ij}^{SC} \neq 0 \) as long as holons are Bose-condensed. At finite temperature, even though the Kosterlitz-Thouless transition temperature for hard-core bosons can be much higher, the “phase coherence” in \( \Delta_{ij}^{SC} \) can be more quickly destroyed at a lower temperature due to the dissolution of the vortices and antivortice bindings in \( \Phi_i^b \) after free spinons appear. Here the argument for \( \langle e^{\pm \Phi_i^b} e^{\pm \Phi_j^b} \rangle = 0 \) is similar to the previous one for \( \langle e^{\Phi_i^b} \rangle = 0 \) which corresponds the disappearance of the long-range AF order once holons become mobile in the metallic phase. This provides us an estimate of the upper limit for the superconducting transition temperature \( T_c \) below.

2. An estimate of \( T_c \)

The holon effective Hamiltonian \( H_h \) in \( \) determines the interaction between holons and those vortices described by \( A_{ij}^h \). If free vortices are few, the condensed holons may easily “screen” them by forming supercurrent, which will then effectively keep \( \Delta_{ij}^{SC} \) finite. But if the number of free vortices, or excited spinons, becomes comparable to the number of holons themselves, one expects that the “screening” effect collapses and thus \( \Delta_{ij}^{SC} = 0 \). It predicts that \( T_c \) will be basically determined by the spinon energy scale in the following way:

\[
2 \sum_{m \neq 0} \frac{\lambda_m}{E_m} n(E_m) \bigg|_{T=T_c} = \kappa N \delta_i,
\] (3.13)

where \( \kappa \sim 1 \) and the left-hand side represent the average number of excited spinons in \( \sum_{ij} b_i^\dagger b_j^\dagger \) with the Bose-condensed part (if exists) excluded. The dashed line in Fig. 3 represents the \( T_c \)’s determined by \( \) in the limit \( \delta \Phi \to 0 \). This curve may be regarded as represents the “optimized” \( T_c \), because with introducing the flux fluctuations, \( \delta \Phi \neq 0 \), there is a finite density of states of spinons emerging at lower energy which effectively reduces \( T_c \) defined in \( \). In the “optimized” limit of \( \delta \Phi = 0 \), one may further simplify Eq.\( \) by only retaining the contribution from the lowest-peak (which has a degeneracy \( \delta N/2 \)) and obtains:

\[
T_c = \frac{1}{c} E_s,
\] (3.14)

where \( c \) is given by

\[
c = \ln \left( 1 + \frac{2}{\kappa} \sqrt{1 + (\xi_s/E_s)^2} \right) > 1.
\] (3.15)

Here \( E_s \) and \( \xi_s \) are the energies of \( E_m \) and \( \xi_m \), respectively, corresponding to the lowest-energy peak shown in Fig. 4 at \( \delta \Phi = 0 \). Therefore, \( T_c \) is indeed determined by the characteristic energy \( E_s \) of spinon excitations.
3. d-wave symmetry of the order parameter: phase string effect

Finally, let us briefly discuss the symmetry of the order parameter $\Delta_{j}^{SC}$. Basically, one needs to compare the relative phase of $\Delta_{j}^{SC}$ between $j = i + \hat{x}$ and $j = i + \hat{y}$, or the phase change of the quantity $\tilde{h}_{j}^{\lambda} \equiv h_{j}^{\lambda} e^{i \mathbf{A}_{j}}$ in (3.12). Imagine that we move a holon from $j = i + \hat{x}$ to $i + \hat{y}$ via site $i + \hat{x} + \hat{y}$. At each step the holon has to exchange positions with a spinon with index $\sigma'$ at site $j'$ which leads to an extra phase $\sigma' \equiv \pm 1$ due to $e^{i \mathbf{A}_{j}}$ in $\tilde{h}_{j}^{\lambda}$. Even though other spinons outside the path also contribute to, say, $\tilde{h}_{i+\hat{x}+\hat{y}} - \tilde{h}_{i+\hat{x}}$, but their effect is canceled out as $h_{j}$ picks up the same phase change but with opposite sign in $H_{h}$. Therefore, in the end $\tilde{h}_{j}^{\lambda}$ acquires a total phase $\sigma' \cdot \sigma_{i+\hat{x}+\hat{y}}$ which is just the phase string on such a path. Its contribution is always negative on average for a short-ranged AF state. Assuming that this is the dominant path, one then concludes that $\Delta_{j}^{SC}$ has to change sign from $j = i + \hat{x}$ to $i + \hat{y}$, namely, the d-wave symmetry. If only the nearest-neighbor-site electron pairing is considered, the order parameter in the momentum space can be written in the form $\Delta_{j}^{SC}(\mathbf{k}) \propto (\cos k_{x}a - \cos k_{y}a)$. Therefore, the nonrepairable phase string effect and AF correlations are directly responsible for the d-wave symmetry of the superconducting condensation in the background of $\Delta^{a} \neq 0$.

D. Experimental implications: dynamic spin susceptibility

1. Local spin dynamic susceptibility

The dynamic spin susceptibility function $\chi''_{L}(\omega) = 1/N \sum_{i} \chi''_{zz}(i; i; \omega)$ describes the on-site spin dynamics and is derived in Appendix as follows

$$\chi''_{L}(\omega) = \frac{\pi}{N} \sum_{m,m' \neq 0} \left( \sum_{\sigma} |w_{m}\sigma(i)|^{2} |w_{m'}\sigma(i)|^{2} \right) \cdot \left[ \frac{\text{sgn}(\omega)}{2} (1 + n(E_{m}) + n(E'_{m}))(u_{m}^{2}v_{m'}^{2} + v_{m}^{2}u_{m'}^{2}) \delta(|\omega| - E_{m} - E_{m'}) + (n(E_{m}) - n(E'_{m}))(u_{m}^{2}v_{m'}^{2} + v_{m}^{2}u_{m'}^{2}) \delta(\omega + E_{m} - E_{m'}) \right],$$

(3.16)

where the summation $\sum'$ only runs over those $m$'s with $\xi_{m} < 0$ (note that $E_{m}$ is symmetric under $\xi_{m} \rightarrow -\xi_{m}$). If there is a Bose condensation of spinons, the contribution from the condensed part to $\chi''_{L}$ may be explicitly sorted out as

$$\chi''_{L}(\omega) = \text{sgn}(\omega) \left( \frac{\pi}{2} n_{BC}^{b} \right) \frac{1}{N} \sum_{m} K_{0m} \frac{\lambda_{m}}{E_{m}} \delta(\omega - E_{m}),$$

(3.17)

with $K_{0m} \equiv N \sum_{i} |w_{m}\sigma(i)|^{2} |w_{m}\sigma(i)|^{2}$ where the subscript 0 refers to the $E_{m} = 0$ state.

Based on Eq. (3.16), two kinds of mean-field solutions, with and without Bose condensation of spinons, will be studied below. Without loss of generality, we consider these two cases at $\delta = 0.143$ in which the corresponding density of states, $\rho_{s}(\omega)$, is already shown in Fig. 4 for both cases. Let us firstly focus on the lowest peak of $\rho_{s}(E)$ shown in Fig. 4. The contribution of such a peak to $\chi''_{L}(\omega)$ was previously discussed in Ref. [18] and is illustrated in Fig. 5 by the lowest sharp peak (dashed line) for $\delta \phi = 0$ and the lowest twin peaks (solid curve) for $\delta \phi = 0.3 \phi$, respectively. One sees two very distinct features here. For the case of $\delta \phi = 0.3 \phi$, there is a Bose condensation contribution at $T < T_{BC} \sim 0.21J$ and it leads to a double-peak structure. But in $\delta \phi = 0$ case, the Bose condensation is absent and one finds only a single sharp peak at $2E_{s} \sim 0.4J$. In other words, $\chi''_{L}(\omega)$ has drastically different characteristics for cases with and without a spinon Bose condensation.

The twin-peak splitting may be understood as follows. The second peak corresponds a pair of spinons excited from the RVB vacuum, while the first peak describes a single spinon excitation as the other branch of spinon is in the Bose-condensate state. Such a lowest-peak basically maps out the lowest peak of the spinon density of states $\rho_{s}(E)$ in Fig. 4 according to (3.17), and the second peak in $\chi''_{L}(\omega)$ is located at an energy approximately twice larger than the first one. The latter one will be always around at low temperature no matter whether there is a Bose condensation or not. So there is a distinct behavior of those two peaks at different temperature as shown in Ref. [18], where the weight of the lowest one gradually diminishes as the temperature approaches to $T_{BC}$.

In contrast, there is only one sharp “resonance-like” peak left in the where the Bose condensation is absent. It corresponds to a pair of spinon excitations located at the lowest peak ($E_{s} \sim 0.2J$) of $\rho_{s}$ in Fig. 4 with $\delta \phi = 0$ (dashed
curve). Note that this is the limit where the flux fluctuating part $\delta A_{ij}^h$ is totally suppressed such that a real spinon gap is opened up at low-energy as shown in Fig. 4. The location of the “resonance” peak, $2E_s$, is slightly lowered in energy as compared to the corresponding (second) peak in the twin-peak case at $\delta \phi = 0.3 \bar{\phi}$. The energy scale of this peak ($2E_s \sim 0.4 \bar{J}$) at $\delta \phi \to 0$ limit is roughly independent of $J_h$ and thus of $t$. This is because $J_h$ term only shifts $\lambda$ to $\lambda_m$ by a constant if there is no dispersion in $\xi_m$ near the lowest (highest) peak, which will not affect $E_m$ near the lowest peak as $\lambda$ will readjust its value correspondingly.

2. Underdoping vs. optimal-doping

We have previously discussed the Bose condensation of spinons and argued that it exists only in an “underdoped” regime. We have also shown that holons as bosons can experience a Bose condensation at $T_c$, leading to the superconducting condensation. If the Bose condensation temperature for holons is higher than $T_{BC}$ for spinons, i.e., $T_c > T_{BC}$, the holons will become Bose-condensed before spinons do and it will be generally a uniform state since there is no inhomogeneous spin ordering above $T_{BC}$. Thus one may have $A_{ij}^h \approx A_{ij}^h$ with $\delta \phi$ being much less than in the normal state. In this case, the Bose condensation of spinons can be effectively prevented at lower temperature because a homogeneous $A_{ij}^h$ generally leads to an opening of a real spinon gap as shown in Fig. 4 for $\phi = 0$. So to be self-consistent, once $T_c > T_{BC}$, $T_{BC}$ may no longer exist and $T_c$ becomes the only meaningful temperature scale. Furthermore, we have already seen that $T_c$ is also optimized under $\delta \phi \sim 0$. Therefore, this region may be properly defined as the “optimal-doping” regime in our theory in contrast to the previously defined underdoped regime at $T_{BC} > T_c$.

Such an optimal-doping phase is charge homogenous and the Bose condensation of spinons is absent. It is characterized, below $T_c$, by the “resonance-like” peak emerging in $\chi''_L(\omega)$ at $2E_s$ in Fig. 5. It is in accord with the 41meV peak found in the optimally doped $YBa_2Cu_3O_7$ below $T_c$, if one chooses $J = 100meV$ here. Above $T_c$, the “resonance” peak will quickly disappear as the motion of holons becomes incoherent and a different behavior of $A_{ij}^h$ is involved as discussed in Sec. II.

On the other hand, the underdoping regime with $T_{BC} > T_c$ is characterized by a low-energy twin-peak structure in $\chi''_L(\omega)$ at $T < T_{BC}$. In contrast to the “optimal-doping” case, such an energy structure may not be qualitatively changed even when $T$ is below $T_c$, as holons are also expected to be condensed inhomogeneously in favor of the spinon energy. A twin-peak feature has been observed recently in the underdoped $YBa_2Cu_3O_{6.5}$ compound by neutron scattering in the odd symmetry channel. In the experiment, the lowest peak is located near 30meV and the second one is near 60meV, indeed about twice bigger in energy. Most recently, in the underdoped $YBa_2Cu_3O_{6.6}$, a second energy scale near 34meV has also been indicated besides the earlier report of the lower energy peak near 70meV. It is noted that the energy scales shown in Fig. 5 are generally doping dependent, and those energies in $YBa_2Cu_3O_{6.5}$ are expected to be relatively smaller than the corresponding peaks in $YBa_2Cu_3O_{6.6}$.

A word of caution about the comparison with the $YBCO$ compound is that the latter is a double-layer system where two adjacent layer coupling is also important. But we do not expect the double-layer coupling to qualitatively change the above energy structure of $\chi''_L$ in the odd symmetry channel. We point out that the fluctuating part of the gauge-field $\delta A_{ij}^h$ usually makes the two adjacent layers difficult to couple together unless there are AF spin domains in the charge deficient region where the total $A_{ij}^h$ is suppressed, as may be the case of phase separation. But in the uniform phase, with $\delta A_{ij}^h$ being suppressed below $T_c$ due to the Bose condensation of holons, the effective coupling between layers can also be greatly enhanced to gain interlayer-coupling spin energy. The Anderson’s confinement-deconfinement phenomenon may become most prominently in the optimal-doping regime, which needs to be further explored.

3. Prediction

Fig. 5 also shows $\chi''_L(\omega)$ in the whole energy regime at $\delta \phi/\bar{\phi} = 0$ (dashed curve) and 0.3 (solid curve), respectively. As compared to the $\delta = 0$ curve in the insert, a multi-peak structure is present as well at high energies for such a doped case. For example, if the 41meV peak in $YBa_2Cu_3O_7$ is explained by the lowest peak in the case of $\delta \phi = 0$, then the theory predicts a second “resonance” peak near 120meV to be found. Those high energy peaks in Fig. 5 become rather closer in energy especially in the Bose condensed case (solid curve) which could be very easily smeared out either by the experimental solution (it may be further complicated by the fact that the momentum-dependence varies drastically among those peaks) or by the dynamic broadening due to the finite life time of spinons which is
beyond the present mean-field treatment. Nevertheless, the multi-peak structure, especially the twin-peak feature at low energy in the spinon Bose-condensed case, should become observable by high solution measurement at low temperature as the unique prediction of the present theory.

IV. DISCUSSIONS

In this paper, we have approached the doped antiferromagnet from the half-filling side, where the bosonic RVB description is known to be very accurate for the antiferromagnetism. The crucial modification at finite doping comes from the phase string effect induced by doped holes. For example, doped holes are turned into bosonic holons by such a phase string effect so that both the elementary spin and charge excitations are bosonic. The Bose condensation of spinons in insulating phase and the Bose condensation of holons in metallic phase determine the AFLRO and superconducting phase transitions, respectively.

While the bosonic RVB pairing, representing short-range AF correlations, is always present and is the driving force behind the antiferromagnetism and superconductivity, it is the combination with the phase string effect that decides when and where they occur in the phase diagram. For instance, the Bose-condensation of spinons leads to the AFLRO only in the case that holes are localized. In the metallic phase where holes become mobile, the AFLRO will be destroyed by the phase string effect. But the Bose-condensation of spinons may still persist into weakly doped metallic region, leading to an “underdoping” metallic phase with charge inhomogeneity (phase separation) and pseudo-gap phenomenon.

There still are many theoretical and experimental issues which have not been dealt with in the present paper and are left for further investigation. Here we conclude by giving several critical remarks. The first is about the phase diagram at larger doping. Recall that in our mean-field description, the metallic phases are characterized by two temperature scales: $T_c$ and $T_{BC}$, and we have argued that $T_c > T_{BC}$ determines an “optimal-doping” regime at low temperature where $T_{BC}$ is no longer meaningful. But beyond this regime, there is a possibility that holons may tend to be always Bose-condensed even at normal state in favor of the hopping energy. If this occurs, the gauge field $A^f_{ij}$ in $H_f$ may have to be “expelled” to the spinon part, leading to a statistics transmutation to turn spinons into fermions and causing a collapse of the bosonic RVB order parameter at the normal state. In this picture, the normal state in overdoped regime may simply recover the fermionic uniform RVB state.

The second issue is about the time-reversal symmetry. Recall that the sharp peak structure in spinon spectrum below $T_c$ is mathematically similar to a Landau level structure in a uniform magnetic field. One may naturally wonder if some kind of time-reversal symmetry would be apparently broken like in the anyon theories. Below we point out that this is not the case in the present theory. First of all, it is easy to see that there is no breaking of the time-reversal symmetry in the holon Hamiltonian $H_h$ (2.53) in which the gauge field $A^f_{ij} = A^s_{ij} - φ^0_{ij}$. Here $A^s_{ij}$ behaves like a fluctuating gauge field with $⟨A^s_{ij}⟩ = 0$, and $φ^0_{ij}$ describes a uniform $π$-flux per plaquette which does not break the time-reversal symmetry either as a gauge transformation can easily change $π$ flux into $−π$ flux per plaquette. As for the spin part, even though spinons see $A^s_{ij}$ which breaks the time-reversal symmetry, one should remember that the physical observable quantity is the spin-spin correlation functions like $χ''_{LL}$ shown in (3.10), which can be easily shown to be invariant under $A^f_{ij} → -A^f_{ij}$.

Lastly, the sharp peak in the spinon spectrum in the uniform phase provides an explanation for the 41meV peak in the neutron-scattering measurement of $YBaCuO” 90 K”$ sample, but it also means a real gap in the spinon spectrum. From a naive spin-charge separation picture, one would expect the single-electron Green’s function to be a convolution of spinon and holon propagators and the electron spectrum may also show a finite gap as well in the superconducting state which may be inconsistent with d-wave symmetry. But we note that in the present spin-charge separation formalism (2.13), there is an additional phase field $θ^{string}$ representing the phase string effect. It means that if a “bare” hole created by $c_{id}$ decays into mobile spinon and holon, a nonlocal topological effect will be left behind which could cost a logarithmic-divergent energy. In other words, the phase string effect in 2D case will serve as a confinement force to prevent a newly doped hole from dissolving into elementary excitations. (Of course, internal charge and spin excitations without involving the change of total electron number are still described by the spin-charge separation in the present mean-field theory.) In fact, even in 1D case, the single-electron Green’s function looks quite differently from a simple convolution of spinon and holon propagators, and recently Suzuura and Nagaosa have discussed the crucial role of the phase string effect in understanding the angle-resolved photoemission spectroscopy in $SrCuO_2$. Our preliminary investigation in 2D indicates that a bare “hole” wavepacket injected into the background of the spin-charge separation mean-field state will behave more like a conventional band-structure quasiparticle in a Fermi liquid which shows d-wave gap structure when the holons are Bose-condensed and pseudo-gap structure when
where \( \chi_{n\beta}(i; i; \omega_n) = \int d\tau e^{i\omega_n \tau} \langle T_\tau S^\alpha_i(\tau)S^\beta_i(0) \rangle, \) \( (A1) \)

where \( \omega_n = \frac{2\pi n}{\beta} \). In the following we will determine the dynamic spin susceptibility function \( \chi''_{\alpha\beta}(i; i; \omega) \) based on the present mean-field theory.

Consider \( \langle T_\tau S^\alpha_i(\tau)S^\beta_i(0) \rangle \) in \( \alpha = \beta = \tau \) case. In the present mean-field formulation, one has

\[
\langle T_\tau S^\alpha_i(\tau)S^\beta_i(0) \rangle = \frac{1}{4} \sum_{\sigma \sigma'} \langle T_\tau b^\dagger_{i \sigma}(\tau) b_{i \sigma'}(\tau) b_{i \sigma'}(0) b_{i \sigma}(0) \rangle
\]

\[
= \frac{1}{4} \sum_\sigma \left\langle T_\tau b^\dagger_{i \sigma}(\tau) b_{i \sigma}(0) \right\rangle \left\langle T_\tau b_{i \sigma}(\tau) b^\dagger_{i \sigma}(0) \right\rangle. \quad (A2)
\]

In terms of \( \langle 2.47 \rangle \) and \( \langle 2.58 \rangle \), one has

\[
b^\dagger_{i \sigma}(\tau) \equiv e^{H_{\tau \tau} b^\dagger_{i \sigma} e^{-H_{\tau \tau}} = \sum_m \left( u_m \gamma^\dagger_{m \sigma} e^{E_{m \tau}} - v_m \gamma_{m - \sigma} e^{-E_{m \tau}} \right) w^*_m(i) e^{-i\sigma \chi_m}. \quad (A3)
\]

Then by noting \( w^*_m = w_{m\sigma} \) and that for each \( m \) with \( \xi_m < 0 \), one always can find a state \( \bar{m} \) with \( \xi_{\bar{m}} = -\xi_m > 0 \) with a wavefunction

\[
w_{\bar{m}\sigma}(i) = (-1)^i w_{m\sigma}(i) \quad (A4)
\]

according to \( \langle 2.32 \rangle \), we get

\[
\langle T_\tau b^\dagger_{i \sigma}(\tau) b_{j \sigma}(0) \rangle_{\tau>0} = 2 \sum_m' w^*_m(i) w_{m\sigma}(i) \left[ u_m^2 n(E_m) e^{E_m \tau} + v_m^2 (1 + n(E_m)) e^{-E_m \tau} \right], \quad (A5)
\]

where the summation \( \sum_m' \) only runs over those states with \( \xi_m < 0 \). Then it is straightforward to obtain \( \chi_{zz} \) after integrate out \( \tau \) in \( \langle A3 \rangle \):

\[
\chi_{zz}(i; i; i\omega_n) = \chi^{(+)\tau}_{zz}(i; i; i\omega_n) + \chi^{(+)\tau}_{zz}(i; i; i\omega_n), \quad (A6)
\]

where \( \chi^{(+)\tau}_{zz} \) is defined by

\[
\chi^{(+)\tau}_{zz}(i; i; i\omega_n) = \frac{1}{2} \sum_{mm'} K^{zz}_{mm'}(i, i) \left[ (p_{mm'})^2 \frac{n(E_{m'}) - n(E_m)}{i\omega_n + E_m - E_{m'}} \right.

\[\left. + (i_{mm'})^2 (1 + n(E_m) + n(E_{m'})) \right] \left( \frac{1}{i\omega_n + E_m - E_{m'}} - \frac{1}{i\omega_n - E_m - E_{m'}} \right) \quad (A7)
\]
with

\[ K_{mm'}^{zz}(i, i) \equiv \sum_{\sigma} |w_{m\sigma}(i)|^2 |w_{m'\sigma}(i)|^2. \]  

(A8)

Here the coherent factors, \( p_{mm'}^{\pm} \) and \( t_{mm'}^{\pm} \) are defined by

\[ p_{mm'}^{\pm} = u_m u_{m'} \pm v_m v_{m'}, \]
\[ t_{mm'}^{\pm} = u_m v_{m'} \pm v_m u_{m'}. \]  

(A9)

Finally, the dynamic spin susceptibility function \( \chi''_{zz}(i, i; \omega) \) can be obtained as the imaginary part of \( \chi_{zz} \) after an analytic continuation \( i\omega_n \to \omega + i0^+ \) is made:

\[ \chi''_{zz}(i, i; \omega) = \Phi^{(-)}_{zz}(i, i; \omega) + \Phi^{(+)}_{zz}(i, i; \omega), \]  

(A10)

where

\[ \Phi^{(\pm)}_{zz}(i, i; \omega) = \frac{\pi}{4} \sum_{mm'} K_{mm'}^{zz}(i, i) \left[ (1 + n(E_m) + n(E_{m'})) \left( t_{mm'}^{\pm}\right)^2 \text{sgn}(\omega) \right. \]
\[ \quad \cdot \delta(|\omega| - E_m - E_{m'}) + 2 (n(E_m) - n(E_{m'})) \left( p_{mm'}^{\pm}\right)^2 \delta(\omega + E_m - E_{m'}). \]  

(A11)

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Fig. 1 A sequence of sign mismatches (with reference to a spin background satisfying the Marshall sign rule) left by the hopping of a hole from site $a$ to site $b$ on square lattice.

Fig. 2 Fictitious $\pi$ flux-tubes bound to holons which can only be seen by spinons and are described by the gauge field $A^h_{ij}$ defined by $(2.11)$.

Fig. 3 Phase diagram of the bosonic RVB state characterized by the order parameter $\Delta^s$ (solid curve). Within this phase, the shaded curve sketches a region where a Bose condensation of spinons (BC) occurs, which leads to the AFLRO in an insulating phase (dotted curve) but a charge inhomogeneity with short-ranged spin ordering in metallic region which defines an underdoped regime. Superconducting condensation (SC) happens due to the Bose condensation of holons and $T_c$ (dashed curve) is determined under an optimal condition (see the text).

Fig. 4 Spinon density of states at $\delta = 0.143$ and $T = 0$. Solid curve corresponds to $\delta\phi = 0.3\bar{\phi}$ and the dashed curve is for $\delta\phi = 0$. Insert: the density of states at half-filling. The energy is in units of $J$.

Fig. 5 Local dynamic spin susceptibility versus energy at $\delta = 0.143$. Solid curve: $\delta\phi = 0.3\bar{\phi}$ and dashed curve: $\delta\phi = 0$ at $T = 0$. Note that the lowest peak of dashed curve splits into a twin-peak structure in solid curve (see text). The half-filled case is shown in the insert for comparison.
Fig. 3

$0.0 \quad 0.1 \quad 0.2 \quad 0.3$

$\delta$

$\Delta^s \neq 0$

$T$

BC

SC
Fig. 4
\[ \chi''(\omega) \]

\[ \delta = 0.143 \]

\[ \delta = 0 \]

Fig. 5