

Mean-field description of the 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 the 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 the 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 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.

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I. INTRODUCTION

The t - J Hamiltonian is one of the simplest nontrivial models describing how doped holes move on the antiferromagnetic (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 method¹ 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 resonating-valence-bond (RVB) states,² gauge-theory description,^{3,4} $\text{SU}(2)$ formalism,⁵ to possible fractional statistics.^{6,7} 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 rule⁸ (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 wave function 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 the serious problem of an 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^{9,10} and its mean-field version—the Schwinger-boson mean-field approach¹¹—in describing spin properties at half-filling. A variational wave function based on the bosonic RVB picture can produce^{9,10} an unrivaled accurate ground-state energy ($-0.3344J$ per bond as com-

pared to the exact numerical value of $-0.3346J$ per bond for the Heisenberg model), and a generalized description¹⁰ can precisely produce not only the ground-state energy, staggered magnetization, but also spin-excitation spectrum in the whole Brillouin zone. Therefore, a bosonic description of spins seems most natural at half-filling.

It is thus tempting for one to use the bosonic description of spins as a starting point and to try to get into the metallic phase by doping. The connection between antiferromagnetic and metallic phases is commonly perceived important in the t - J model, and is also believed by many to be the key in search for the mechanism of superconductivity in cuprates. Unfortunately, the mean-field study in the Schwinger-boson-slave-fermion approach¹² of the t - J model, which is based on the bosonic description of spins and has been quite successful at half-filling,¹¹ soon meets problematic consequences once holes are introduced—encountering the so-called spiral phase and its derivatives.^{13,14} It seems that one could not avoid such a spiral instability so long as a perturbative approach is adopted.¹⁵ One of many problems with spiral phases involves an underestimated kinetic energy $\propto \delta^2(t^2/J)$ at weak doping $\delta \ll 1$, which is also accompanied by a very quick descent to ferromagnetic phase at slightly larger δ .¹⁴

This implies that doped holes may have introduced some *singular* doping effect which has been mistreated in the mean-field approximations. Such a singular doping effect has been recently identified^{16,17} by reexamining the 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.¹⁶ 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 transformation¹⁷ 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 reformulation¹⁷ 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^{12,14} 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 reproduced¹⁷ after a mean-field decoupling of the spin and charge degrees of freedom in this scheme.

In this paper, we develop a generalized mean-field-type theory based on this formalism of the t - J model in the two-dimensional (2D) case. This theory recovers the well-known Schwinger-boson mean-field state¹¹ 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 AF long-range-order (LRO) phase, an underdoped metallic phase with the phenomena of pseudogap 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.¹⁸

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

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

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

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

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

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

and the superexchange term is

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

Note that the staggered phase factor $(-\sigma)^i$ in Eq. (2.1) is introduced¹⁷ to explicitly track the Marshall sign, which leads to the negative sign in Eq. (2.4). A sign $\sigma = \pm 1$ then

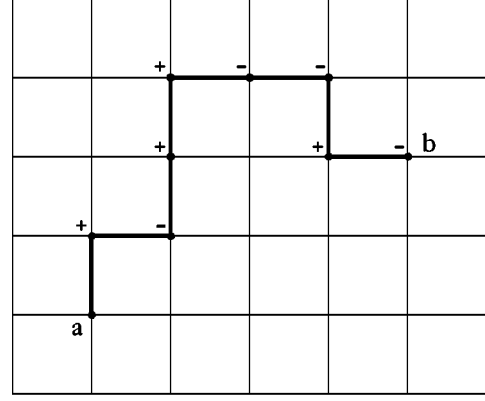


FIG. 1. A sequence of sign mismatches (with reference to a spin background satisfying the Marshall sign rule) left by the hopping of a hole from site a to site b on square lattice.

appears in the hopping term (2.3) which is the origin of the phase string effect^{16,17} mentioned in the Introduction. Due to such a sign, a hole moving from a site a to another site b will acquire a sequence of signs, i.e., a phase string as shown in Fig. 1, which has been shown^{16,17} 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 the 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.¹⁷ The resulting formalism is known as the phase string representation. The hopping term H_t in this representation becomes¹⁷

$$H_t = -t \sum_{\langle ij \rangle \sigma} (e^{iA_{ij}^f}) h_i^\dagger h_j (e^{i\sigma A_{ji}^h}) b_{j\sigma}^\dagger b_{i\sigma} + \text{H.c.}, \quad (2.5)$$

and the superexchange term H_J reads

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

Note that the fermionic operator f_i now is replaced by a *bosonic* holon operator h_i in this 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:

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

In this formalism, the singular phase string effect, as represented by the sign σ 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}^f and A_{ij}^h . These fields are defined as follows:

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

with

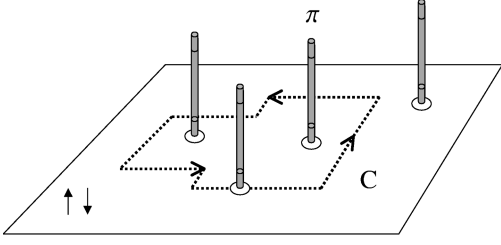


FIG. 2. Fictitious π flux tubes bound to holons which can only be seen by spinons and are described by the gauge field A_{ij}^h defined by Eq. (2.11).

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

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

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 $n_{i\sigma}^b$ and n_i^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 ϕ_{ij}^0 describes a uniform flux threading through the 2D plane with a strength π per plaquette: $\sum_{\square} \phi_{ij}^0 = \pm \pi$. It is also noted that a π -flux neutral topological excitation has been previously discussed¹⁹ 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.

The electron operator in this representation becomes¹⁷

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

Here the nonlocal phase factor $e^{i\Theta_{i\sigma}^{\text{string}}}$ precisely keeps the track of the singular part of the phase string effect and is defined by

$$\Theta_{i\sigma}^{\text{string}} \equiv \frac{1}{2} [\Phi_i^b - \sigma \Phi_i^h], \quad (2.14)$$

with

$$\Phi_i^b \equiv \sum_{l \neq i} \theta_i(l) \left(\sum_{\alpha} \alpha n_{l\alpha}^b - 1 \right), \quad (2.15)$$

and

$$\Phi_i^h \equiv \sum_{l \neq i} \theta_i(l) n_l^h. \quad (2.16)$$

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 introduced by Arovas and Auerbach.¹¹ Such a mean-field is characterized by a bosonic RVB order parameter

$$\Delta^s = \sum_{\sigma} \langle b_{i\sigma} b_{j-\sigma} \rangle \quad (2.17)$$

for the nearest-neighbor sites i and j [$i = \text{NN}(j)$].

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,

$$\Delta_{ij}^s = \sum_{\sigma} \langle e^{-i\sigma A_{ij}^h} b_{i\sigma} b_{j-\sigma} \rangle. \quad (2.18)$$

Δ_{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 Eq. (2.6) in a standard procedure

$$\begin{aligned} H_s^J = & -\frac{J}{2} \sum_{\langle ij \rangle \sigma} (\Delta_{ij}^s)^* e^{-i\sigma A_{ij}^h} b_{i\sigma} b_{j-\sigma} + \text{H.c.} \\ & + \frac{J}{2} \sum_{\langle ij \rangle} |\Delta_{ij}^s|^2 + \lambda \left(\sum_{i\sigma} b_{i\sigma}^{\dagger} b_{i\sigma} - (1 - \delta)N \right), \end{aligned} \quad (2.19)$$

where the last term with a Lagrangian multiplier λ is introduced to enforce the condition of total spinon number, with N denoting the total lattice number and δ doping concentration. In order to diagonalize H_s^J , we introduce the following Bogoliubov transformation:

$$b_{i\sigma} = \sum_m (u_{m\sigma}(i) \gamma_{m\sigma} - v_{m\sigma}(i) \gamma_{m-\sigma}^{\dagger}), \quad (2.20)$$

and seek the solution

$$[H_s^J, \gamma_{m\sigma}^{\dagger}] = E_m \gamma_{m\sigma}^{\dagger}, \quad (2.21)$$

$$[H_s^J, \gamma_{m\sigma}] = -E_m \gamma_{m\sigma}. \quad (2.22)$$

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 σ . 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 Eq. (2.19), we have

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

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

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

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

We can further express $u_{m\sigma}(i)$ and $v_{m\sigma}(i)$ by the ‘‘one-particle’’ wave function $w_{m\sigma}(i)$ 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 Eq. (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 eigenequation for the one-particle wave function $w_{m\sigma}$:

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

The eigenvalue ξ_m in Eq. (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 λ_m is the same as the Lagrangian multiplier λ , but we write it in a general form because later it will be modified once the hopping term is introduced. In terms of Eqs. (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 $\text{sgn}(v_m/u_m) = \text{sgn}(\xi_m)$. As a convention we will always choose $u_m = |u_m|$ and $v_m = |v_m| \text{sgn}(\xi_m)$.

Thus H_s^J is diagonalized as $H_s^J = \sum_{m\sigma} E_m \gamma_{m\sigma}^\dagger \gamma_{m\sigma} + \text{const}$ according to Eqs. (2.21) and (2.22). The order parameter Δ_{ij}^s can be self-consistently determined by the definition (2.18) as

$$\Delta_{ij}^s = \sum_{m\sigma} e^{-i\sigma A_{ij}^h} w_{m\sigma}(i) w_{m-\sigma}(j) (-u_m v_m) \times \left[1 + \sum_{\alpha} \langle \gamma_{m\alpha}^\dagger \gamma_{m\alpha} \rangle \right]. \quad (2.37)$$

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

$$\sum_{\langle ij \rangle} |\Delta_{ij}^s|^2 = \sum_m \frac{\xi_m^2}{J E_m} \coth \frac{\beta E_m}{2}, \quad (2.38)$$

with $\langle \gamma_{m\sigma}^\dagger \gamma_{m\sigma} \rangle = 1/(e^{\beta E_m} - 1)$ and $\beta \equiv 1/k_B T$. Finally, the condition

$$\left\langle \sum_{i\sigma} b_{i\sigma}^\dagger b_{i\sigma} \right\rangle = (1 - \delta)N, \quad (2.39)$$

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

$$2 - \delta = \frac{1}{N} \sum_{m \neq 0} \frac{\lambda_m}{E_m} \coth \frac{\beta E_m}{2} + n_{\text{BC}}^b, \quad (2.40)$$

where n_{BC}^b is introduced to describe the contribution from the $E_m = 0$ 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 ξ_m and wave function $w_{m\sigma}(i)$]. One may simply recover the Schwinger-boson mean-field results by setting $A_{ij}^h = 0$ in Eq. (2.32) and obtaining $\xi_k = -J\Delta_0^s (\cos k_x a + \cos k_y a)$ and the Bloch wave function $w_{k\sigma} = (1/\sqrt{N}) e^{i\sigma \mathbf{k} \cdot \mathbf{r}_i}$ 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 Eq. (2.39); the other is through the gauge field A_{ij}^h . For the mean-field theory to work, A_{ij}^h has been implicitly assumed as a time-independent field. But with holons moving around, A_{ij}^h will usually gain a dynamic effect. To see this, let us consider the following gauge-invariant quantity:

$$\sum_C A_{ij}^h = \pi \sum_{l \in C} n_l^h, \quad (2.41)$$

where C is an arbitrary counterclockwise closed path. If one redefines

$$n_i^h = \delta + \delta n_i^h \quad (2.42)$$

with $\delta n_i^h = n_i^h - \delta$, then correspondingly

$$A_{ij}^h = \bar{A}_{ij}^h + \delta A_{ij}^h, \quad (2.43)$$

where

$$\sum_C \bar{A}_{ij}^h = \pi \delta \frac{S_c}{a^2} \equiv \bar{\phi} \frac{S_c}{a^2}, \quad (2.44)$$

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

$$\sum_C \delta A_{ij}^h = \pi \sum_{l \in C} \delta n_l^h. \quad (2.45)$$

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 δA_{ij}^h on the spinon part at the mean-field level and replace it by some random flux fluctuations with a strength per plaquette equal to $\delta\phi$ [One may estimate $\delta\phi \approx \pi \sqrt{(\delta n^h)^2}$]. This can be justified at low temperature when a Bose condensation of holons (which corresponds to a superconducting condensation as shown later) occurs, where δA_{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 δA_{ij}^h can dominate over \bar{A}_{ij}^h and the separation of the latter from 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 π 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 wave function $w_{m\sigma}(i)$ 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.,

$$w_{m\sigma}(i) \rightarrow e^{i\sigma\chi_m} w_{m\sigma}(i), \quad (2.46)$$

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

$$b_{i\sigma} = \sum_m (u_m \gamma_{m\sigma} - v_m \gamma_{m-\sigma}^\dagger) e^{i\sigma\chi_m} w_{m\sigma}(i). \quad (2.47)$$

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 Eq. (2.5). By using the Bogoliubov expression for spinon operators, a straightforward calculation gives

$$\left\langle \sum_\sigma e^{i\sigma A_{ji}^h} b_{j\sigma}^\dagger b_{i\sigma} \right\rangle = \sum_{m\sigma} e^{i\sigma A_{ji}^h} w_{m\sigma}^*(j) w_{m\sigma}(i) e^{-i\sigma\Delta\chi_m} \times [v_m^2 + (u_m^2 + v_m^2) \langle \gamma_{m\sigma}^\dagger \gamma_{m\sigma} \rangle]. \quad (2.48)$$

Note that $\Delta\chi_m$ in the above expression denotes the difference of χ_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 Eq. (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 Eq. (2.32) with an eigenvalue $\xi_m^- = -\xi_m$ and the cancellation in Eq. (2.48) stems from the fact that those quantities like u_m^2 and v_m^2 only depend on E_m in Eq. (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:

$$e^{i\sigma\chi_m} \rightarrow [-\text{sgn}(\xi_m)] \times e^{i\sigma\chi_m}, \quad (2.49)$$

or

$$e^{-i\sigma\Delta\chi_m} = -\text{sgn}(\xi_m). \quad (2.50)$$

Then, one finds

$$\begin{aligned} B_0 &\equiv \frac{1}{2N} \sum_{\langle ij \rangle \sigma} \langle e^{i\sigma A_{ji}^h} b_{j\sigma}^\dagger b_{i\sigma} \rangle \\ &= \frac{1}{2N} \sum_{m\sigma} B_m^0 [v_m^2 + (u_m^2 + v_m^2) \langle \gamma_{m\sigma}^\dagger \gamma_{m\sigma} \rangle], \end{aligned} \quad (2.51)$$

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

$$\begin{aligned} B_m^0 &= -\text{sgn}(\xi_m) \sum_{\langle ij \rangle} e^{i\sigma A_{ji}^h} w_{m\sigma}^*(j) w_{m\sigma}(i) \\ &= \text{sgn}(\xi_m) (\xi_m / 2J_s) \sum_i w_{m\sigma}^*(i) w_{m\sigma}(i) = \frac{|\xi_m|}{2J_s} > 0. \end{aligned} \quad (2.52)$$

In obtaining the second line above, we have used Eq. (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

$$H_h = -t_h \sum_{\langle ij \rangle} e^{iA_{ij}^f} h_i^\dagger h_j + \text{H.c.}, \quad (2.53)$$

which is derived from H_t with an effective hopping integral

$$t_h \equiv t B_0. \quad (2.54)$$

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 Eq. (2.3) will always lead to $t_h = 0$ and make a spiral twist (an order parameter in favor of hole hopping) necessary in any local mean-field treatment.

Finally, to be consistent, the hopping effect *on* spinons is obtained from H_t as

$$H_s^t = -J_h \sum_{\langle ij \rangle \sigma} e^{i\sigma A_{ji}^h} b_{j\sigma}^\dagger b_{i\sigma} + \text{H.c.} + 4J_h B_0 N, \quad (2.55)$$

in which $J_h \equiv \langle e^{iA_{ij}^f} h_i^\dagger h_j \rangle t \propto \delta t$ measures the strength of hopping effect on the spinon part. [The constant in Eq. (2.55) is introduced such that $\langle H_s^t \rangle = 0$.] Hence the total Hamiltonian describing spinon degrees of freedom is composed of two terms

$$H_s = H_s^J + H_s^t, \quad (2.56)$$

where H_s^J in Eq. (2.19) has been diagonalized at the mean-field level before. H_s^t can be expressed in terms of Eq. (2.47) by noting that $b_{j\sigma}^\dagger$ and $b_{i\sigma}$ in Eq. (2.55) should differ by a phase shift Eq. (2.49) as a holon switches sublattice sites. It then gives

$$H_s^t = -J_h \sum_{m\sigma} B_m^0 (u_m \gamma_{m\sigma}^\dagger - v_m \gamma_{m-\sigma}) (u_m \gamma_{m\sigma} - v_m \gamma_{m-\sigma}^\dagger) + \text{H.c.} + 4J_h B_0 N, \quad (2.57)$$

after using the orthogonal condition $\sum_i w_{m\sigma}^*(i) w_{m'\sigma}(i) = \delta_{m,m'}$ as well as Eq. (2.32). On the other hand, one has $H_s^J = \sum_{m\sigma} E_m \gamma_{m\sigma}^\dagger \gamma_{m\sigma} + \text{const}$ (note that $\lambda_m = \lambda$ inside E_m here). Then H_s can be diagonalized in a straightforward way. If we are still to use E_m to denote the spinon spectrum for the sake of compactness, then H_s can be finally written as

$$H_s = \sum_{m\sigma} E_m \gamma_{m\sigma}^\dagger \gamma_{m\sigma} + E_0^s, \quad (2.58)$$

where

$$E_0^s = -2 \sum_m E_m n(E_m) - \frac{J}{2} \sum_{\langle ij \rangle} |\Delta_{ij}^s|^2. \quad (2.59)$$

But here the spinon spectrum

$$E_m = \sqrt{\lambda_m^2 - \xi_m^2} \quad (2.60)$$

is different from the previous one obtained in previous section by a correction to λ_m due to the hopping effect:

$$\lambda_m = \lambda - \frac{J_h}{J_s} |\xi_m|. \quad (2.61)$$

Therefore, the hopping effect on the spinon part is *solely* represented by a shift from λ to λ_m in Eq. (2.61). The Bogoliubov transformation (2.61) remains unchanged and so do u_m and v_m defined in Eqs. (2.35) and (2.36), so long as the renormalized λ_m is used. The Lagrangian multiplier λ in Eq. (2.61) is still determined by Eq. (2.40) where both λ_m and E_m should be replaced by the renormalized ones in Eqs.

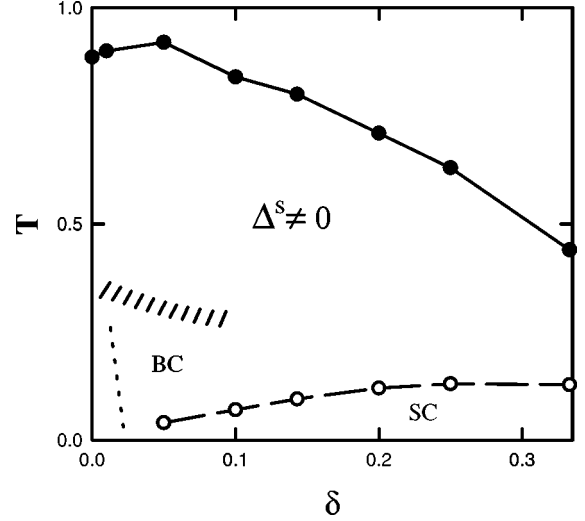


FIG. 3. Phase diagram of the bosonic RVB state characterized by the order parameter Δ^s (solid curve). Within this phase, the shaded curve sketches a region where a Bose condensation of spinons (BC) occurs, which leads to the AFLRO in an insulating phase (dotted curve) but a charge inhomogeneity with 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).

(2.60) and (2.61). Finally, the self-consistent equation (2.38) for the RVB pairing order parameter maybe rewritten as

$$\Delta^s = \frac{1-2\delta}{4N} \sum_m \frac{\xi_m^2}{J_s E_m} \coth \frac{\beta E_m}{2}. \quad (2.62)$$

[Note that if the Bose condensation occurs, one may separate the contribution from the condensation part on the right-hand side by $\Delta_{\text{BC}}^s \equiv (1-2\delta) |\xi_0|^2 n_{\text{BC}}^b / 4J_s \lambda_0$.] In obtaining Eq. (2.62), we have used an approximate relation

$$1/(2N) \sum_{\langle ij \rangle} \langle (\Delta_{ij}^s)^2 \rangle_h \approx \Delta^{s2} / (1-2\delta)$$

at $\delta \ll 0.5$ limit. Such a relation can be obtained by assuming $\Delta_{ij}^s = \Delta_1^s$ when i and j belongs to occupied sites and $\Delta_{ij}^s = 0$ if i or j is at hole site and by noting that each hole accounts for $\Delta_{ij}^s = 0$ at four adjacent bonds at dilute-hole limit which leads to $\Delta^s = (1-2\delta) \Delta_1^s$.

III. PHASE DIAGRAM

A. Unified bosonic RVB phase

Our mean-field theory has been constructed based on a single bosonic RVB order parameter Δ^s . Such an order parameter controls short-range spin-spin correlations in *both* the undoped and doped regime. Figure 3 shows a typical region of $\Delta^s \neq 0$ obtained by solving the mean-field equations which has been briefly discussed in Ref. 18. It obviously covers the whole experimentally interested temperature (from $T=0$ to $T \sim 0.5 - 0.9J/k_B$) 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 Δ^s does not directly correspond to an energy gap, in contrast to the fermionic RVB theory¹ (the latter is similar to the BCS theory in mathematical structure). Also note that the crossover from $\Delta^s \neq 0$ phase to $\Delta^s = 0$ phase at high temperature is similar to the half-filling case¹¹ which does not correspond to a real phase transition.

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

Although $\Delta^s \neq 0$ 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 condensation²⁰ of spinons. Such a Bose condensation of spinons, as represented by $n_{BC}^b \neq 0$ in Eq. (2.40), describes a long-range AF spin ordering.²⁰ 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 expression (2.13), spin operators, S_i^z and S_i^\pm , can be easily written down in terms of spinon operator $b_{i\sigma}$ after using the constraint (2.7):

$$S_i^z = \frac{1}{2} \sum_{\sigma} \sigma b_{i\sigma}^\dagger b_{i\sigma}, \quad (3.1)$$

and

$$S_i^+ = b_{i\uparrow}^\dagger b_{i\downarrow} (-1)^i e^{i\Phi_i^h} \quad (3.2)$$

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

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

$$\langle S_i^+ \rangle \propto (-1)^i, \quad (3.3)$$

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

$$\langle e^{i\Phi_i^h} \rangle = 0. \quad (3.4)$$

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

$$\theta_i(l) \rightarrow \theta_i(l) + \phi \quad (3.5)$$

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

$$e^{i\Phi_i^h} \rightarrow e^{i\Phi_i^h} \times e^{i\phi N^h}. \quad (3.6)$$

Here N^h is the total holon number. Thus the average of such a phase must vanish at finite doping as given in Eq. (3.4). Since Φ_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 frustration effect of phase string becomes ineffective, may the AFLRO 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, Φ_i^h in S_i^+ can be effectively canceled out by the opposite vorticities generated from spinons. After all, the topological (Berry’s phase) effect of the phase string is no longer there if holes cannot complete a closed path at large length scale. In this insulating phase, the phase string effect may play a crucial role *causing* the localization of holes. We expect such an insulating phase to exist only at a very dilute density of holons at the expense of the latter’s kinetic energy.

2. Bose condensation of spinons in metallic phase: Underdoping

We have shown that the AFLRO must be absent in the metallic phase. One may naturally wonder if the Bose condensation of spinons can still persist into the 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 inset). Here $\rho_s(E)$ is defined by

$$\rho_s(E) = \frac{1}{N} \sum_m \delta(E - E_m). \quad (3.7)$$

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 ξ_m which, as the solution of Eq. (2.40), has a Hofstadter structure (or the Landau levels in the continuum limit) due to a uniform flux ($\bar{\phi} = \pi\delta$ per plaquette) represented by the vector potential \bar{A}_{ij}^h threading through the square lattice. The broadening of the solid curve in Fig. 4 is due to the redistribution of eigen-

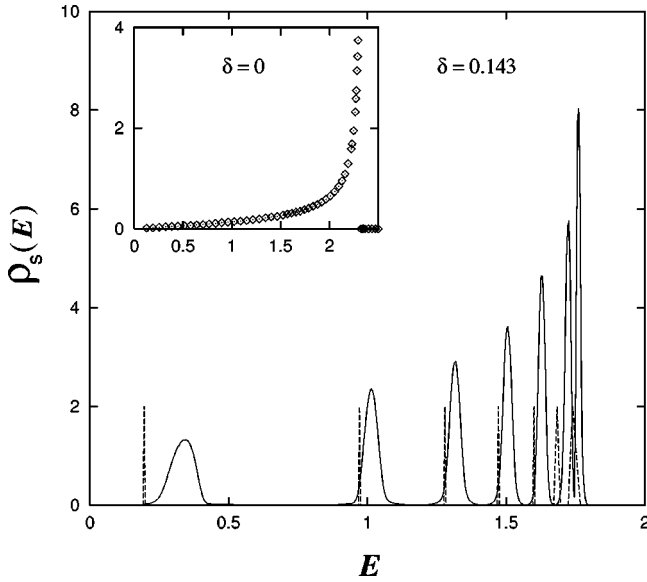


FIG. 4. Spinon density of states at $\delta=0.143$ and $T=0$. The solid curve corresponds to $\delta\phi=0.3\bar{\phi}$ and the dashed curve is for $\delta\phi=0$. Inset: the density of states at half-filling. The energy is in units of J .

states under the fluctuating flux δA_{ij}^h , which is treated as a random flux (in the white-noise limit), here with a maximum strength chosen at $\delta\phi=0.3\bar{\phi}$ 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 $\delta\phi=0.3\bar{\phi}$ (but not at $\delta\phi=0$) as the solution of Eq. (2.40). Recall that the spinon Bose condensation stems from Eq. (2.40) with a nonzero n_{BC}^b representing the density of spinons staying at the $E_m=0$ state. In this case, there would be no solution at low temperature unless λ takes a value to make E_m gapless such that $n_{\text{BC}}^b \neq 0$ can balance the difference between the left and right side of the equation, similar to the half-filled case.²⁰ In particular, such a Bose condensation is found to be sustained up to a finite temperature $T_{\text{BC}} \sim 0.21J$ 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 δA_{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 $\bar{\xi}_m$. So due to the Bose condensation, such quantum states will acquire a macroscopic meaning. But these band-edge states of $\bar{\xi}_m$ 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 $\bar{\xi}_m$ can be close to $\pm 2J_s$. Since the probability would be small for such kinds 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 appear as 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.

Pseudogap behavior. The Bose condensation of spinons will also lead to a pseudogap phenomenon. In the 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 pseudospin 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 pseudogap 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 the metallic phase, it will result in a phase-separation or spin pseudogap phase without the AFLRO. With the increase of δ , the reduction of the left-hand side of Eq. (2.40) will eventually make the Bose condensation term, if initially exists, disappear from the right-hand side. So the Bose condensation in general may only exist at the 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

$$\hat{\Delta}_{ij}^{\text{SC}} \equiv \sum_{\sigma} \sigma c_{i\sigma} c_{j-\sigma} \quad (3.8)$$

can be expressed in terms of Eq. (2.13) as follows:

$$\hat{\Delta}_{ij}^{\text{SC}} = \hat{\Delta}_{ij}^s (h_i^\dagger e^{(i/2)\Phi_i^b}) (h_j^\dagger e^{(i/2)\Phi_j^b}) (-1)^i, \quad (3.9)$$

in which

$$\hat{\Delta}_{ij}^s \equiv \sum_{\sigma} e^{-i\sigma A_{ij}^h} b_{i\sigma} b_{j-\sigma}. \quad (3.10)$$

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-neighbor pairing with $i = \text{NN}(j)$ below. Since the whole mean-field phase is built on

$$\langle \hat{\Delta}_{ij}^s \rangle = \Delta^s \neq 0, \quad (3.11)$$

the electron pairing order parameter $\Delta_{ij}^{\text{SC}} = \langle \hat{\Delta}_{ij}^{\text{SC}} \rangle$ can be written as

$$\Delta_{ij}^{\text{SC}} = \Delta^s \langle (h_i^\dagger e^{(i/2)\Phi_i^b})(h_j^\dagger e^{(i/2)\Phi_j^b}) \rangle (-1)^i. \quad (3.12)$$

We see that the spinons are always paired in the present phase, as described by Δ^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-field theory.⁴ But there are two crucial differences.

First, 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.

Second, 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 fluctuations⁴) to bring down the temperature scale in the slave-boson mean-field approximation. On the other hand, there is a unique feature in Eq. (3.12), namely, the presence of phases like $e^{(i/2)\Phi_i^b}$. Here Φ_i^b represents a structure of vortices (antivortices) 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 antivortices in Φ_i^b , which implies $\Delta_{ij}^{\text{SC}} \neq 0$ 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 Δ_{ij}^{SC} can be more quickly destroyed at a lower temperature due to the dissolution of the vortices and antivortice bindings in Φ_i^b after *free* spinons appear. Here the argument for $\langle e^{(i/2)\Phi_i^b} e^{(i/2)\Phi_j^b} \rangle = 0$ is similar to the previous one for $\langle e^{i\Phi_i^h} \rangle = 0$ 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 Eq. (2.53) 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 Δ_{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 $\Delta_{ij}^{\text{SC}} = 0$. It predicts that T_c will be basically determined by the spinon energy scale in the following way:

$$2 \sum_{m \neq 0} \frac{\lambda_m}{E_m} n(E_m) \Big|_{T=T_c} = \kappa N \delta, \quad (3.13)$$

where $\kappa \sim 1$ and the left-hand side represent the average number of excited spinons in $\sum_{i\sigma} b_{i\sigma}^\dagger b_{i\sigma}$ with the Bose-condensed part (if exists) excluded. The dashed line in Fig. 3 represents the T_c 's determined by Eq. (3.13) in the limit $\delta\phi \rightarrow 0$. 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 Eq. (3.13). In the ‘‘optimized’’ limit of $\delta\phi = 0$, one may further simplify Eq. (3.13) by only retaining the contribution from the lowest-peak (which has a degeneracy $\delta N/2$) and obtains

$$T_c = \frac{1}{c} E_s, \quad (3.14)$$

where c is given by

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

Here E_s and ξ_s are the energies of E_m and ξ_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 Δ_{ij}^{SC} . Basically, one needs to compare the relative phase of Δ_{ij}^{SC} between $j = i + \hat{x}$ and $j = i + \hat{y}$, or the phase change of the quantity $\tilde{h}_j^\dagger \equiv h_j^\dagger e^{(i/2)\Phi_j^b}$ in Eq. (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 $\sigma_{j'}$ at site j' which leads to an extra phase $\sigma_{j'} = \pm 1$ due to $e^{(i/2)\Phi_j^b}$ in \tilde{h}_j^\dagger . Even though other spinons outside the path also contribute to, say, $\Phi_{i+\hat{x}+\hat{y}}^b - \Phi_{i+\hat{x}}^b$, 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^\dagger acquires a total phase $\sigma_{i+\hat{y}} \cdot \sigma_{i+\hat{x}+\hat{y}}$ 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 Δ_{ij}^{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 $\Delta^{\text{SC}}(\mathbf{k}) \propto (\cos k_x a - \cos k_y a)$. 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 $\Delta^s \neq 0$.

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 the Appendix as follows:

$$\begin{aligned} \chi_L''(\omega) = & \frac{\pi}{N} \sum_{mm'}' \left(\sum_{i\sigma} |w_{m\sigma}(i)|^2 |w_{m'\sigma}(i)|^2 \right) \\ & \times \left[\frac{\text{sgn}(\omega)}{2} (1 + n(E_m) + n(E_{m'})) \right. \\ & \times (u_m^2 v_{m'}^2 + v_m^2 u_{m'}^2) \delta(|\omega| - E_m - E_{m'}) \\ & + [n(E_m) - n(E_{m'})] (u_m^2 u_{m'}^2 + v_m^2 v_{m'}^2) \\ & \left. \times \delta(\omega + E_m - E_{m'}) \right], \end{aligned} \quad (3.16)$$

where the summation Σ' 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 χ_L'' may be explicitly sorted out as

$$\chi_c''(\omega) = \text{sgn}(\omega) \left(\frac{\pi}{2} n_{\text{BC}}^b \right) \frac{1}{N} \sum_m' K_{0m} \frac{\lambda_m}{E_m} \delta(\omega - E_m), \quad (3.17)$$

with $K_{0m} \equiv N \sum_{i\sigma} |w_{0\sigma}(i)|^2 |w_{m\sigma}(i)|^2$ 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 first 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 $\delta\phi = 0.3\bar{\phi}$, respectively. One sees two very distinct features here. For the case of $\delta\phi = 0.3\bar{\phi}$, there is a Bose condensation contribution at $T < T_{\text{BC}} \sim 0.21J$ 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 to a pair of spinons excited from the RVB vacuum, while the first peak describes a *single* spinon excitation as the other branch of the spinon is in the

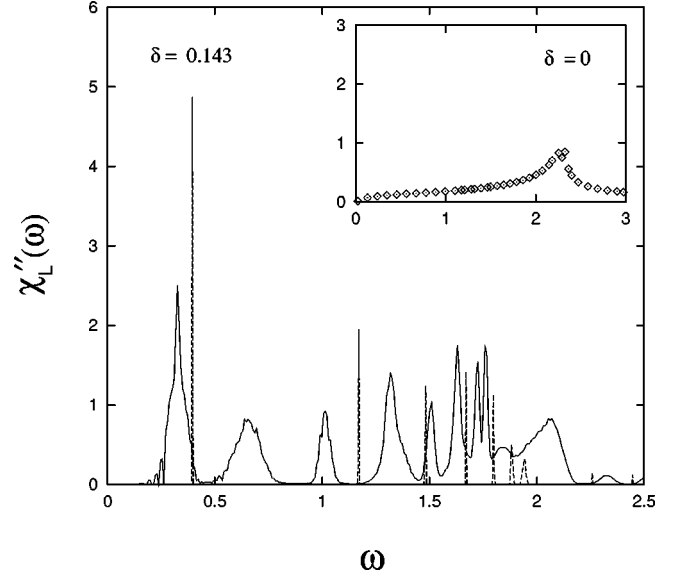


FIG. 5. Local dynamic spin susceptibility versus energy at $\delta = 0.143$. Solid curve: $\delta\phi = 0.3\bar{\phi}$ and the dashed curve: $\delta\phi = 0$ at $T = 0$. Note that the lowest peak of dashed curve splits into a twin-peak structure in the solid curve (see text). The half-filled case is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

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 Eq. (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 T_{BC} .

In contrast, there is only one sharp “resonancelike” 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 ρ_s in Fig. 4 with $\delta\phi = 0$ (dashed curve). Note that this is the limit where the flux fluctuating part δA_{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 ($2E_s \sim 0.4J$) at $\delta\phi \rightarrow 0$ limit is roughly independent of J_h and thus of t . This is because the J_h term only shifts λ to λ_m by a const if there is no dispersion in ξ_m near the lowest (highest) peak, which will not affect E_m near the lowest peak as λ 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., $T_c > T_{\text{BC}}$, the holons will become Bose condensed before spinons do and it will be generally a *uniform* state since there is no inhomoge-

neous spin ordering above T_{BC} . Thus one may have $A_{ij}^h \approx \bar{A}_{ij}^h$ 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 \bar{A}_{ij}^h generally leads to an opening of a real spinon gap as shown in Fig. 4 for $\delta\phi=0$. 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 homogeneous and the Bose condensation of spinons is absent. It is characterized, below T_c , by the ‘‘resonancelike’’ peak emerging in $\chi_L''(\omega)$ at $2E_s$ in Fig. 5. It is in accord with the 41 meV peak found²² in the optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_7$ below T_c , if one chooses $J=100$ meV 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 $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ compound by neutron scattering²³ in the odd symmetry channel. In the experiment, the lowest peak is located near 30 meV and the second one is near 60 meV, indeed about twice bigger in energy. Most recently, in the underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$, a second energy scale near ~ 70 meV has been also indicated²⁴ besides the earlier report of the lower energy peak near 34 meV.²⁵ It is noted that the energy scales shown in Fig. 5 are generally doping dependent, and those energies in $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$ are expected to be relatively smaller than the corresponding peaks in $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$.

A word of caution about the comparison with the Y-Ba-Cu-O 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 χ_L'' in the odd symmetry channel. We point out that the fluctuating part of the gauge-field δA_{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 in phase separation. But in the uniform phase, with δA_{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 phenomenon²⁶ may become most prominently in the optimal-doping regime, which needs to be further explored.

3. Prediction

Figure 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 inset, a multipeak structure is present as well at high energies for such a doped case. For example, if the 41 meV peak in $\text{YBa}_2\text{Cu}_3\text{O}_7$ is explained by the lowest peak in the case of $\delta\phi=0$, then the theory predicts a second ‘‘resonance’’ peak near 120 meV 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 lifetime of spinons which is beyond the present mean-field treatment. Nevertheless, the multipeak structure, especially the twin-peak feature at low energy in the spinon Bose-condensed case, should become observable by high resolution 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 the insulating phase and the Bose condensation of holons in the 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 the weakly doped metallic region, leading to an ‘‘underdoping’’ metallic phase with charge inhomogeneity (phase separation) and pseudogap 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 the *normal state* in favor of the hopping energy. If this occurs, the gauge field A_{ij}^f in H_J 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 the overdoped regime may simply recover the fermionic uniform RVB state.⁴

The second issue is about the time-reversal symmetry. Recall that the sharp peak structure in the 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.⁶ 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 $A_{ij}^f = A_{ij}^s - \phi_{ij}^0$. Here A_{ij}^s behaves like a fluctuating gauge field with $\langle A_{ij}^s \rangle = 0$, and ϕ_{ij}^0 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 $-\pi$ flux per plaquette. As for the spin part, even though spinons see A_{ij}^h which breaks the time-reversal symmetry, one should remember that the physical observable quantity is the spin-spin correlation functions like χ_L'' shown in Eq. (3.16), which can be easily shown to be invariant under $A_{ij}^h \rightarrow -A_{ij}^h$. It is also straightforward to check that the spin chirality²⁹ characterized by $\langle \mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3) \rangle$ is always zero by using the condition $w_{m-\sigma}^*(i) = w_{m\sigma}(i)$.

Lastly, the sharp peak in the spinon spectrum in the uniform phase provides an explanation for the 41 meV peak in the neutron-scattering measurement of Y-Ba-Cu-O ‘‘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-shift field $\Theta_{i\sigma}^{\text{sing}}$ representing the phase string effect. It means that if a ‘‘bare’’ hole created by $c_{i\sigma}$ decays into a 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 the 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 the total electron number are still described by the spin-charge separation in the present mean-field theory.) In fact, even in the 1D case, the single-electron Green’s function looks quite differently from a simple convolution of spinon and holon propagators, and recently Suzuura and Nagaosa²⁷ have discussed the crucial role of the phase string effect in understanding the angle-resolved photoemission spectroscopy in SrCuO₂.²⁸ The phase-shift field $\Theta_{i\sigma}^{\text{sing}}$ also plays a role in recovering the ‘‘large’’ Fermi surface as discussed in Ref. 17 for 1D. Our preliminary investigation in 2D indicates that a bare ‘‘hole’’ wave packet 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 with a large Fermi surface, which shows *d*-wave gap structure when the holons are Bose condensed and pseudogap structure when spinons are Bose condensed. So experiments involving injecting an electron or a hole into the system, like photoemission spectroscopy, may no longer provide *direct* information of elementary excitations like in the conventional

Fermi-liquid theory, due to the confinement of the phase string effect.

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APPENDIX: DYNAMIC SPIN SUSCEPTIBILITY FUNCTION

Local spin susceptibility function is defined in the Matsubara representation as follows:

$$\chi_{\alpha\beta}(i, i; i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} \langle T_\tau S_i^\alpha(\tau) S_i^\beta(0) \rangle, \quad (\text{A1})$$

where $\omega_n = 2\pi n/\beta$. 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 $\langle T_\tau S_i^\alpha(\tau) S_i^\beta(0) \rangle$ in $\alpha = \beta = z$ case. In the present mean-field formulation, one has

$$\begin{aligned} & \langle T_\tau S_i^z(\tau) S_i^z(0) \rangle \\ &= \frac{1}{4} \sum_{\sigma\sigma'} \sigma\sigma' \langle T_\tau b_{i\sigma}^\dagger(\tau) b_{i\sigma}(\tau) b_{i\sigma'}^\dagger(0) b_{i\sigma'}(0) \rangle \\ &= \frac{1}{4} \sum_{\sigma} \langle T_\tau b_{i\sigma}^\dagger(\tau) b_{i\sigma}(0) \rangle \langle T_\tau b_{i\sigma}(\tau) b_{i\sigma}^\dagger(0) \rangle. \end{aligned} \quad (\text{A2})$$

In terms of Eqs. (2.47) and (2.58), one has

$$\begin{aligned} b_{i\sigma}^\dagger(\tau) &\equiv e^{H_s\tau} b_{i\sigma}^\dagger e^{-H_s\tau} \\ &= \sum_m (u_m \gamma_{m\sigma}^\dagger e^{E_m\tau} - v_m \gamma_{m-\sigma} e^{-E_m\tau}) w_{m\sigma}^*(i) e^{-i\sigma\chi_m}. \end{aligned} \quad (\text{A3})$$

Then by noting $w_{m-\sigma}^* = w_{m\sigma}$ 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 wave function

$$w_{\bar{m}\sigma}(i) = (-1)^i w_{m\sigma}(i), \quad (\text{A4})$$

according to Eq. (2.32), we get

$$\begin{aligned} & \langle T_\tau b_{i\sigma}^\dagger(\tau) b_{j\sigma}(0) \rangle_{\tau>0} \\ &= 2 \sum_m' w_{m\sigma}^*(i) w_{m\sigma}(i) \times \{ u_m^2 n(E_m) e^{E_m\tau} \\ & \quad + v_m^2 [1 + n(E_m)] e^{-E_m\tau} \}, \end{aligned} \quad (\text{A5})$$

where the summation \sum_m' only runs over those states with $\xi_m < 0$. Then it is straightforward to obtain χ_{zz} after integrating out τ in Eq. (A2):

$$\chi_{zz}(i, i; i\omega_n) = \chi_{zz}^{(-)}(i, i; i\omega_n) + \chi_{zz}^{(+)}(i, i; i\omega_n), \quad (\text{A6})$$

where $\chi_{zz}^{(\pm)}$ is defined by

$$\begin{aligned} \chi_{zz}^{(\pm)}(i, i; i\omega_n) &= \frac{1}{2} \sum'_{mm'} K_{mm'}^{zz}(i, i) \\ &\times \left[(p_{mm'}^{\pm})^2 \frac{n(E_{m'}) - n(E_m)}{i\omega_n + E_m - E_{m'}} \right. \\ &+ (l_{mm'}^{\pm})^2 [1 + n(E_m) + n(E_{m'})] \\ &\left. \times \frac{1}{2} \left(\frac{1}{i\omega_n + E_m + E_{m'}} - \frac{1}{i\omega_n - E_m - E_{m'}} \right) \right] \end{aligned} \quad (\text{A7})$$

with

$$K_{mm'}^{zz}(i, i) \equiv \sum_{\sigma} |w_{m\sigma}(i)|^2 |w_{m'\sigma}(i)|^2. \quad (\text{A8})$$

Here the coherent factors, $p_{mm'}^{\pm}$, and $l_{mm'}^{\pm}$, are defined by

$$\begin{aligned} p_{mm'}^{\pm} &= u_m u_{m'} \pm v_m v_{m'}, \\ l_{mm'}^{\pm} &= u_m v_{m'} \pm v_m u_{m'}. \end{aligned} \quad (\text{A9})$$

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

$$\chi_{zz}''(i, i; \omega) = \Phi_{zz}^{(-)}(i, i; \omega) + \Phi_{zz}^{(+)}(i, i; \omega), \quad (\text{A10})$$

where

$$\begin{aligned} \Phi_{zz}^{(\pm)}(i, i; \omega) &= \frac{\pi}{4} \sum'_{mm'} K_{mm'}^{zz}(i, i) \{ [1 + n(E_m) + n(E_{m'})] \\ &\times (l_{mm'}^{\pm})^2 \text{sgn}(\omega) \delta(|\omega| - E_m - E_{m'}) \\ &+ 2[n(E_m) - n(E_{m'})] (p_{mm'}^{\pm})^2 \\ &\times \delta(\omega + E_m - E_{m'}) \}. \end{aligned} \quad (\text{A11})$$

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