Competition and possible coexistence of flux and resonating-valence-bond phases in the t - J model

Dong-Ning Sheng,* Zhao-Bin Su, and Lu Yu

*Institute of Theoretical Physics, Chinese Academy of Sciences, P.O. Box 2735, Beijing 100080, China
and International Centre for Theoretical Physics, P.O. Box 586 34100 Trieste, Italy*

(Received 24 July 1990)

The competition and possible coexistence of the flux phase and pairing states are considered within the slave-boson approach. In addition to the gauge-field coupling holons and spinons, a statistical gauge field is introduced to account for the hard-core nature of holons. Using the equivalence of π -uniform and -staggered fluxes, we show the possibility of reducing the staggered flux and guaranteeing the commensurability condition of the uniform flux for holons at the same time. For certain dopings the frustration of the spinon gauge field to holon motion can be compensated by the holon's own statistical gauge field. Contrary to earlier conclusions of other authors, we find that the flux phase can coexist with the resonating-valence-bond (RVB) states below a critical doping concentration δ_c , beyond which the d -wave RVB state takes over.

The t - J model has been extensively studied in connection with high- T_c superconductivity. Various quantum-liquid states (QLS) including the resonating valence bond (RVB) (Refs. 1-4) as well as several flux phases⁵⁻⁹ have been proposed as candidates for ground states of pristine and doped systems. Due to the local SU(2) symmetry at half filling,³ the d -wave and the $s+id$ RVB (Kotliar²) states as well as the π -flux phase (Affleck and Marston⁵) are degenerate. Within renormalized mean-field theory,⁴ the d -wave state has the lowest kinetic energy for an extra hole ($-2.71t$). This is also true for the π -flux phase. Hence these two states are competitive candidates for the ground state.

In the slave-boson representation the spinons are fermions and cannot all occupy the lowest-energy level. However, by assigning one-half flux quantum per plaquette, one can convert the fermion into a hard-core boson.¹⁰ A natural generalization for the non-half-filled case would still be one flux per particle, i.e., $\Phi/2\pi = \nu$, the filling factor. This is the commensurate flux phase (CFP) (Refs. 8 and 9) which gains the exchange energy. However, the gauge field created by spinons frustrates the holon motion, raising its kinetic energy. Thus the CFP is favored only in the limit $t < J$, which is not the most relevant case for high- T_c superconductors.

The flux penetrating the neighboring plaquettes can alternate in direction to form a staggered flux phase (SFP) which is equivalent to the π -flux phase at half filling. The energy band is split into two subbands touching each other. The mean-field and small-cluster calculations⁹ show that SFP is energetically favored against CFP for $t > J$. Recently, Zhang¹¹ has studied the competition and possible coexistence of the SFP with the d -wave RVB state and has concluded that the SFP is unstable against the d -wave RVB state at all non-half-fillings.

However, Zhang's conclusion is based on the renormalized mean-field theory, which treats the no-double-occupancy constraint only in the average sense. Very recently, Nori, Abarhams, and Zimanyi¹² have shown that, if the hard-core nature of holons is taken into account by

statistics transmutation, the slave-boson mean-field theory allows for a solution where both spinons and holons experience one flux quantum per particle with much lower energy for the uniform flux phase. On the other hand, the pairing instability is not considered in Ref. 12. In this Rapid Communication, we take into account both the hard-core nature of holons and the pairing instability to reexamine the competition and possible coexistence of SFP and RVB states. Using the equivalence of the π -staggered and uniform flux, we can largely compensate the frustration effects of the staggered flux on holon motion by the holon's own uniform statistical flux. In contrast to Zhang, we find a critical doping δ_c below which the SFP coexists with the $s+id$ RVB state, while the d -wave RVB state takes over only beyond it. Over a certain range of doping the spinons are locked into a π -SFP whose frustration to the holon motion is completely compensated by the holon's own statistical gauge field.

We start from the slave-boson representation of the t - J Hamiltonian

$$H = -t_s \sum_{\langle i,j \rangle, \sigma} b_i^\dagger b_j c_{j\sigma}^\dagger c_{i\sigma} + \text{H.c.} - J_s \sum_{\langle i,j \rangle} c_i^\dagger c_j^\dagger (c_{i\downarrow} c_{j\uparrow} + c_{j\downarrow} c_{i\uparrow}) - \mu \sum_{i,\sigma} [c_{i\sigma}^\dagger c_{i\sigma} - (1 - \delta)] + \lambda \sum_i \left(\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} + b_i^\dagger b_i - 1 \right), \quad (1)$$

where $b_i^\dagger(b_i)$ and $c_i^\dagger(c_i)$ are charged boson (holon) and neutral fermion (spinon) creation (annihilation) operators, respectively. Here μ is the chemical potential while λ is the Lagrange multiplier. We have introduced the renormalization of hopping constant $t_s = 2t/(1 + \delta)$ and the exchange interaction $J_s = 4J/(1 + \delta)^2$ to account for the single-occupancy constraint in the average sense⁴ with δ as the doping concentration.

Following Ref. 12, we introduce the statistical gauge field $\hat{A}_{ij}$ defined as $b_i^\dagger b_j = \exp(i\hat{A}_{ij}) h_i^\dagger h_j$, with $h_i^\dagger, h_j$ as fermion operators, while the gauge field $\hat{A}_{ij}$ in the mean-field approximation is given by¹²

$$\sum_{\text{plaquette}} \hat{A}_{ij} = 2\pi(2q + 1)\delta. \quad (2)$$

Consider the following order parameters

$$p \exp(-i\phi_{ij}) = \sum_{\sigma} \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle, \quad (3)$$

$$\Delta_{ij} \equiv \langle (c_{i\downarrow} c_{j\uparrow} - c_{i\uparrow} c_{j\downarrow}) \rangle, \quad (4)$$

$$h_{ij} \equiv \langle e^{i(A_{ij} + \phi_{ij})} h_i^{\dagger} h_j \rangle, \quad (5)$$

where i, j are the nearest neighbors and $\phi_{ij} = \pm \Phi/4$ which satisfies the condition $\phi_{i,i \pm \hat{x}} = -\phi_{i,i \pm \hat{y}} = \phi_{i+\hat{x},i+\hat{x} \pm \hat{y}}, \tau = x, y$. On the other hand, the pairing order parameter depends only on the coordinate direction, i.e., $\Delta_{\tau} = \Delta_{i,i+\hat{\tau}} = \Delta_{i,i-\hat{\tau}}$.

The mean-field Hamiltonian can then be written as

$$H_{\text{MF}} = H_s + H_h + H_c, \quad (6)$$

$$H_s = - \left[\sum_{\langle i,j \rangle, \sigma} \left(t_s h_{ij}^* + \frac{3J_s}{8} p \right) e^{i\phi_{ij}} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{3J_s}{8} \sum_{\langle i,j \rangle, \sigma} \sigma \Delta_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}^{\dagger} \right] + \text{H.c.} - \mu_1 \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma}, \quad (7)$$

$$H_h = -t_s \sum_{\langle i,j \rangle} p \exp[i(A_{ij} + \phi_{ij})] h_i^{\dagger} h_j + \text{H.c.} - \mu_2 \sum_i h_i^{\dagger} h_i, \quad (8)$$

$$H_c = \frac{3NJ_s}{8} (|\Delta_x|^2 + |\Delta_y|^2) - \sum_i \left[\left(t_s h_{i,i+\hat{x}}^* + \frac{3J_s p}{8} \right) p + \left(t_s h_{i,i+\hat{y}}^* + \frac{3J_s p}{8} \right) p \right] + \text{c.c.} - \frac{3J_s}{4} p^2 N + \mu_1 N (1 - \delta) + \mu_2 \delta N, \quad (9)$$

where $\mu_1 = \mu - \lambda$, $\mu_2 = -\lambda$, and N is the number of sites. Taking into account the gauge invariance of $\exp(iA_{ij}) h_i^{\dagger} h_j$ and the symmetry property of ϕ_{ij} , we can replace h_{ij} by its average value $h = (h_{i,i+\hat{x}} + h_{i,i+\hat{y}})/2$ which should be gauge and translationally invariant in the mean-field approximation. Hence we neglect the feedback effect of holon motion on spinons.

Now we solve the mean-field Hamiltonian (6). The spinon part H_s can be diagonalized by the standard procedure to obtain the spinon-free energy F_s as a function of order parameters. As for the holon part H_h , we note that the resulting flux acting on a holon is a superposition of its own statistical gauge field and the flux field created by spinons, i.e.,

$$\begin{aligned} \Phi_h &= \sum_{\text{plaquette}} (A_{ij} + \phi_{ij}) + 2\pi k = 2\pi\delta + 4\pi q\delta + 2\pi k \pm \Phi \\ &= 2\pi\delta + (4\pi q\delta + 2\pi k + \epsilon\pi) \pm (\Phi - \epsilon\pi) = \tilde{B} \pm \tilde{\Phi}, \end{aligned} \quad (10)$$

where k, q are integers and $\epsilon = 0, \pm 1$, and they can be adjusted to minimize the holon energy. The first two terms are the uniform flux $\tilde{B}$ while the last part is the staggered flux $\tilde{\Phi}$. Note that the flux on a lattice is defined up to 2π per plaquette. To lower the holon kinetic energy one has to (i) reduce the staggered flux whose presence narrows the band and raises the energy at small dopings; (ii) minimize the second bracket to satisfy the commensurability condition. These two conditions can be compatible with each other. For example, if $\Phi < \pi/2$, we take $q = k = \epsilon = 0$, while if $\Phi > \pi/2$, we set $\epsilon = 1$ to reduce the staggered flux and then choose appropriate values for q and k , so that $-4\pi\delta < 4\pi q\delta + 2\pi k + \epsilon\pi < 0$, i.e., $|\tilde{B}| = 2\pi\delta\nu$ with $0 < \nu < 1$. This means that holons will behave like anions with ν statistics¹⁰ which will lead to a slight increase of energy, but such a state is still energetically favorable. For doping concentration $\delta = r/p$ with r, p as irreducible positive integers, and assuming the Landau gauge for the vector potential $\vec{A} = \vec{B}(0, x)$, the gauge field of the uniform flux is periodic in the x direction with period $2p$. On the other hand, the staggered field $\tilde{\Phi}$ is

periodic in 2×2 . Hence the holon motion is periodic in $2p \times 2$. This is true if p is an odd integer. Otherwise, $2p$ should be replaced by p . The gauge field $A_{ij} + \phi_{ij}$ in (8) can be replaced by $A_{ij} + \tilde{\phi}_{ij}$ with $\tilde{\phi}_{ij} = \pm \tilde{\Phi}/4$. Considering a supercell of $2p \times 2$ particles and following the procedure of Hasegawa and co-workers⁸ the holon Hamiltonian can also be diagonalized to yield the holon free energy F_h which depends on $\tilde{B}$, $\tilde{\Phi}$, and p .

The total free energy is then the sum $F = F_s + F_h + H_c$ with H_c given by (9). It is an explicit function of p , Δ , μ_1 , μ_2 , h , and Φ , and at the same time depends on $\tilde{B}$ and $\tilde{\Phi}$ which, in turn, are fully determined by Φ for a given doping concentration. Therefore, it is convenient to first solve self-consistent equations for other order parameters and then vary F with respect to Φ to find the genuine minimum.

The effective holon hopping energy

$$\begin{aligned} E_h &= -t_s \sum_{\langle i,j \rangle} \langle p \exp[i(A_{ij} + \phi_{ij})] h_i^{\dagger} h_j \rangle + \text{c.c.} \\ &= -4t_s p h N \end{aligned} \quad (11)$$

can be determined for any given Φ . The parameters ϵ, k, q are chosen by minimizing the holon hopping energy, which will, in turn, also minimize the total free energy, because the spinon energy [see (7)], not depending explicitly on ϵ, k , and q , increases with the order parameter h . The optimal E_h are plotted by solid lines in Fig. 1 for different dopings, while the corresponding curves for $k = q = \epsilon = 0$ are plotted by dashed lines. For the latter case the commensurability condition, i.e., $\tilde{B} = 2\pi\delta$ is satisfied, but the minimization of staggered flux is not guaranteed so that there is a monotonic increase for $\Phi > \pi/2$. This increase, however, can be compensated for certain dopings by choosing $\epsilon = 1$ and appropriate q, k to reduce Φ to $\tilde{\Phi} = \Phi - \pi/2$. In fact, if $\delta = (2p_1 - 1)/4k_1$ with p_1, k_1 as positive integers, by taking $\epsilon = 0$ for $\Phi < \pi/2$ and $\epsilon = 1$ for $\Phi > \pi/2$, both conditions can be satisfied, as shown by solid lines a and f in Fig. 1 for $\delta = \frac{7}{100}$ and $\frac{3}{8}$, respectively. This means that the effect of the π -flux part is compensated by the statistical gauge field without

FIG. 1. The effective holon energy E_h (in units of $t_s p N$) as a function of flux Φ (in units of π). The dashed lines are the results for $\epsilon=0$, while the solid lines are calculated by the optimal choice of ϵ to lower the holon energy. The curves a, b, c, d, e , and f correspond to doping concentrations of $\frac{7}{100}$, $\frac{7}{50}$, $\frac{4}{25}$, $\frac{13}{50}$, $\frac{3}{10}$, and $\frac{3}{8}$, respectively.

changing the hard-core boson nature of holons. On the other hand, if $\delta = (2p_1 - 1)/(4k_1 - 2)$, the two conditions cannot be satisfied at the same time for $\Phi > \pi/2$, i.e., either the staggered flux is not minimized or the holon is transformed from a boson into a fermion. For low concentrations (e.g., curve $b, \delta = \frac{7}{50}$), the effect of the staggered field is more important, so the holon energy is significantly lowered by choosing $\epsilon=1$. However, for higher concentrations the statistics is the dominating factor, so the minimum energy always corresponds to $\epsilon=0$ (see curves $d, \delta = \frac{13}{50}$ and $e, \delta = \frac{3}{10}$, where the dashed and solid lines coincide with each other). For other dopings the holon is transformed into an anion¹⁰ after absorbing the staggered flux π . For $\Phi=\pi, \delta = \frac{4}{25}$ (curve c) the holon is carrying a

FIG. 2. The total free energy F (in units of NJ) as a function of flux Φ (in units of π). Curves a, b, c, d, e , and f correspond to dopings $\frac{7}{100}$, $\frac{7}{50}$, $\frac{4}{25}$, $\frac{13}{50}$, $\frac{3}{10}$, and $\frac{3}{8}$, respectively.

FIG. 3. The comparison of the total free energy F (in units of NJ) for the $\Phi=0$ phase (d -wave RVB, dashed line) and the $\Phi=\pi$ phase (coexisting flux and $s+id$ wave RVB, solid line) as a function of doping concentration δ with a critical concentration δ_c .

uniform flux $\tilde{B} = \pi\delta/4$, so its energy is lower than a bare fermion but higher than a hard-core boson. Anyway, at low concentrations the holon energy can be lowered by combining the staggered flux with the uniform statistical flux.

The total free energy as a function of Φ for different dopings is plotted in Fig. 2. For low dopings the π -flux phase is favored (curves a, b, c), while the no-flux phase wins only at high dopings (curves e, f). Curve d for which the minimum is not at $\Phi=0$ or π , corresponds to the transition region, which is rather narrow. In what follows we will compare only the π -flux phase with the no-flux phase. Figure 3 shows the competition of π -flux phase with d -wave RVB state (zero flux) with a critical value at $\delta_c = 0.275$, below which the π -flux phase is favored while beyond it the d -wave RVB state wins. Here we have set $t/J=5$ and expect δ_c to decrease with t/J . We should also mention that the curve for π -flux phase was calculated using the Fermi statistics for holons. For more general statistics, the coexisting phase would be energetically even more favorable.

Our numerical calculations have shown that the π -flux phase coexists with the $s+id$ RVB state. Due to the $SU(2)$ symmetry, only the flux order parameter is needed at half filling. For nonvanishing δ , this symmetry is broken, so the pairing fluctuation also becomes important which gradually suppresses the preference of the flux phase for the spinon part and eventually overwhelms above δ_c with d -wave pairing. For any flux phase with $\Phi \neq \pi$, the d -wave state is always favored against the s -wave state.

To summarize, by incorporating the gauge field created by spinons and the statistical gauge field of holons due to their hard-core nature, we have shown that the staggered π -flux phase can coexist with the RVB state in the t - J model for low dopings, contrary to the earlier con-

clusion.¹¹ Of course, a pure π -flux phase (without pairing) is one of the flux phases, so its energy may be higher than the optimal CFP. However, the Fermi level is located in the largest gap in CFP which does not favor electron pairing. With the increase of δ , such fluctuations may favor the staggered phase against CFP. Eventually, at

even higher dopings (greater than δ_c), the staggered phase also gives its way to a pure d -wave RVB state.

One of us (Z.B.S.) would like to thank D. H. Lee and C. Kane for helpful discussions.

*Also at the Chinese Center of Advanced Science and Technology (World Laboratory), Beijing, China.

¹G. Baskaran, Z. Zou, and P. W. Anderson, *Solid State Commun.* **63**, 973 (1987).

²G. Kotliar, *Phys. Rev. B* **37**, 3664 (1988).

³I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, *Phys. Rev. B* **38**, 745 (1988).

⁴F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, *Supercond. Sci. Technol.* **1**, 36 (1988).

⁵I. Affleck and J. B. Marston, *Phys. Rev. B* **37**, 3774 (1988).

⁶P. W. Anderson, *Phys. Scr.* **T27**, 60 (1989); P. W. Anderson, B. S. Shastry, and D. Hristopoulos, *Phys. Rev. B* **40**, 8939 (1989).

⁷Y. Hasegawa, P. Lederer, T. M. Rice, and P. B. Wiegmann, *Phys. Rev. Lett.* **63**, 907 (1989).

⁸P. Lederer, D. Poilblanc, and T. M. Rice, *Phys. Rev. Lett.* **63**,

1519 (1989); D. Poilblanc, Y. Hasegawa, and T. M. Rice, *Phys. Rev. B* **41**, 1949 (1990); S. Liang, and N. Trivedi, *Phys. Rev. Lett.* **64**, 232 (1990).

⁹A. B. Harris, T. C. Lubensky, and E. J. Mele, *Phys. Rev. B* **40**, 2631 (1989); D. Poilblanc and Y. Hasegawa, *Phys. Rev. B* **40**, 9035 (1989).

¹⁰S. C. Zhang, T. H. Hansson, and S. A. Kivelson, *Phys. Rev. Lett.* **62**, (1989); E. Fradkin, *ibid.* **63**, 322 (1989); G. Baskaran, in *Two-Dimensional Strongly Correlated Electronic Systems*, edited by Z. Z. Gan and Z. B. Su (Gordon & Breach, Amsterdam, 1989), p. 47.

¹¹F. C. Zhang, *Phys. Rev. Lett.* **64**, 974 (1990).

¹²F. Nori, E. Abrahams, and G. T. Zimanyi, *Phys. Rev. B* **41**, 7277 (1989); see also, J. P. Rodrigues and B. Doucot, *Europhys. Lett.* **11**, 415 (1990).