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The spiral phase and the spin-liquid state in the t–J–J' model

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Abstract. The possible spin-liquid state and phase separation are studied in the framework of the t–J–J' model (frustrated t–J model) by using the Schwinger boson mean-field theory. It is shown that both doping and the quantum fluctuation of spins, which are treated on the same footing, favour the spin-liquid state. Away from half filling, the phase separation is still present for any values of t/J and J'/J in the case of spin $S = \frac{1}{2}$, but a tendency to diminish the range of the phase separation is induced due to quantum fluctuation of the spins.

Very soon after the discovery of the copper oxide superconductors [1] Anderson [2] pointed out that the key to understanding them may lie in their copper oxide sheets (CuO_2), and especially in the exchange interactions between the magnetic moments on the copper ions. Anderson [2] proposed that for small spin values, strong quantum fluctuations may generate a novel spin-liquid (SL) ground state with no long-range order. Anderson [2] and later Zhang and Rice [3] argued strongly that a two-dimensional, large-U, single-band Hubbard model provides a consistent description of the copper oxide sheets. In the large-U limit, the Hubbard model may be transformed into the t–J model

$$H = -t \sum_{\langle ij\rangle\sigma} C^{\dagger}_{i\sigma} C_{j\sigma} + \mathrm{HC} + J \sum_{\langle ij\rangle} (S_i S_j - \tfrac{1}{4} n_i n_j) \qquad (1)$$

acting on the space with no doubly occupied sites, with S_i the electron spin and n_i the electron number, where $C^{\dagger}_{i\sigma}$ creates an electron of spin σ on site i, and the sum over $\langle ij\rangle$ is over nearest neighbours. The Hamiltonian (1) is supplemented by the constraint that there be no doubly occupied sites. In the half-filled case, the t–J model reduces to the Heisenberg Hamiltonian. Away from half filling, the model is characterized by a competition between kinetic energy t and magnetic energy J. The magnetic energy J favours antiferromagnetic (AFM) order for the spins, whereas the kinetic energy t favours delocalization of the holes and tends to destroy the AFM spin order.

Although the t–J model provides a reasonable description for the relationship [4, 5] between doping and antiferromagnetism, it also raises an interesting question about the phase instability. Emery *et al* [6] have argued that, for the t–J model, dilute

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holes in an antiferromagnet are unstable against phase separation into a hole-rich and no-hole phase, and the transition from the ordered state to the doped state is first order. In the mean-field approximation, Wen *et al* [7] argued that for large enough values of frustration, the quantum fluctuation of spins may well melt the AFM order phase, resulting in a chiral SL state. Their argument [7] was based on the J–J' model (the frustrated Heisenberg model), where the effect of doping was not included. The fact of the matter is that AFM order may be destroyed by both quantum fluctuation of spins and doping [8]. Thus a detailed understanding of the motion of 'holes' in a frustrated quantum antiferromagnet is of fundamental importance. In this paper, we present a mean-field calculation to show that the quantum fluctuation of spins is essential in stabilizing the SL state and diminishing the range of the phase separation in the framework of the t–J–J' model (the frustrated t–J model)

$$H = -t\sum_{\langle ij\rangle\sigma} C^\dagger_{i\sigma}C_{j\sigma} + \mathrm{HC} + J\sum_{\langle ij\rangle}(S_iS_j - \tfrac{1}{4}n_in_j) + J'\sum_{il}(S_iS_l - \tfrac{1}{4}n_in_l) \qquad (2)$$

by using Schwinger boson mean-field theory, where the sum over il is over next-nearest neighbours. The primary role of the J' term is to introduce frustration of spins which destabilizes the AFM ordering and favours the SL state with no long-range order [7]. The original t–J model also contains the quantum fluctuation of spins, but the essential quantum fluctuation of spins is due to the frustration term J' in the mean-field approximation [7]. Thus we can treat both the doping and quantum fluctuation of spins on the same footing in the mean-field approximation.

In the Schwinger boson representation [9, 10], the electron operator can be expressed as $C_{i\sigma} = f^\dagger_i b_{i\sigma}$ with the constraint $\sum_\sigma b^\dagger_{i\sigma}b_{i\sigma} + f^\dagger_i f_i = 1$. In this case, the t–J–J' Hamiltonian (2) may be written as

$$\begin{aligned} H = -t\sum_{\langle ij\rangle\sigma} f_i f^\dagger_j b^\dagger_{i\sigma}b_{j\sigma} + \mathrm{HC} - \mu\sum_i f^\dagger_i f_i + \frac{J}{4}\sum_{\langle ij\rangle} b^\dagger_{i\alpha}b_{i\beta}b^\dagger_{j\gamma}b_{j\delta}(\sigma_{\alpha\beta}\sigma_{\gamma\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta}) \\ + \frac{J'}{4}\sum_{il} b^\dagger_{i\alpha}b_{i\beta}b^\dagger_{l\gamma}b_{l\delta}(\sigma_{\alpha\beta}\sigma_{\gamma\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta}) \\ + \sum_i \lambda_i\Big(f^\dagger_i f_i + \sum_\sigma b^\dagger_{i\sigma}b_{i\sigma} - 2S\Big) \end{aligned} \qquad (3)$$

which allows us to treat the double-occupancy-forbidding constraint in a straightforward approximation. Here λ_i is the Lagrangian multiplier on the site i, and μ is the chemical potential. The boson operator, $b^\dagger_{i\sigma}$, keeps track of the spin, while the fermion operator, $f^\dagger_i$, keeps track of the hole. The Schwinger boson mean-field approximation to the Hamiltonian (3) amounts to treating λ_i as a constant independent of position and decoupling the spin interaction in a Hartree-like approximation by introducing the resonating valence bond (RVB) order parameter:

$$D_k = \sum_\eta \mathrm{e}^{ik\eta}D_\eta \qquad (D_\eta \equiv \langle b_{i\uparrow}b_{i+\eta\downarrow} - b_{i\downarrow}b_{i+\eta\uparrow}\rangle)$$

on each bond, where $\eta = \pm x, \pm y$, and the particle–hole amplitude

$$F_k = \sum_\eta \mathrm{e}^{ik\eta}F_\eta \qquad (F_\eta \equiv \langle f^\dagger_i f_{i+\eta}\rangle)$$

and

$$Q_k = \sum_{\eta} e^{ik\eta} Q_\eta \qquad (Q_\eta \equiv \langle b^\dagger_{i\uparrow} b_{i+\eta\uparrow} + b^\dagger_{i\downarrow} b_{i+\eta\downarrow} \rangle)$$

is the order parameter which describes the spiral and other quantum antiferromagnetic states [9], such as the canted and the double-spiral states, since it is non-zero when neighbouring spins have finite overlap.

$$B_k = \sum_{\tau} e^{ik\eta} B_\tau \qquad (B_\tau \equiv \langle b^\dagger_{i\uparrow} b_{i+\tau\uparrow} + b^\dagger_{i\downarrow} b_{i+\tau\downarrow} \rangle)$$

is the order parameter which describes the quantum fluctuation of spins in the present mean-field approximation, where $\tau = \pm x \pm y$.

Kane *et al* [9], and Auerbach and Larson [10] argued that the energy of the state with spiral order is lower than those, such as the canted state or the double-spiral state, for small doping δ in the framework of the t–t'–J model or t–J model, where the Schwinger bosons Bose condense at zero temperature for $S = \frac{1}{2}$, which signifies long-range AFM order [11]. At half filling, the fraction of condensation is $\delta_c \simeq 0.61$. In particular, Auerbach and Larson [10] have shown that the long-range-order spiral state is unstable against phase separation between a hole-rich phase and the no-hole phase. This instability manifests itself at the mean-field level as a negative compressibility. In the following calculations, the purpose is to restudy this question by considering the frustrated term J'. Without loss of generality, we take the order parameter B_τ to have s symmetry, i.e. $B_\tau \equiv B^0$, then for the state [12] where a spiral along the (1,1) direction corresponds to $Q_x = Q_y = -Q_{-x} = -Q_{-y}$, $F_x = F_y = -F_{-x} = -F_{-y}$, $D_x = D_y = D_{-x} = D_{-y}$. In this case, we can obtain the self-consistent equations [9, 10] for λ, D, Q, F, B by minimizing the free energy of the system.

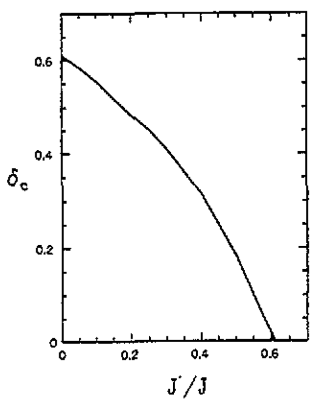

Figure 1. Variation of the Bose condensation fraction δ_c with J'/J at half filling.

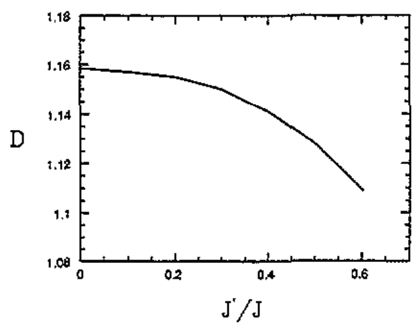

Figure 2. Variation of the RVB order parameter D with J'/J at half filling.

We can now proceed to a brief discussion of our numerical results for the Bose condensation fraction δ_c, and the order parameters. Figure 1 shows that the Bose condensation fraction δ_c, which signifies long-range AFM spiral order [11], decreases with increasing J'/J at half filling. This result is also in agreement with those discussed by Wen *et al* [7]. For a large enough value of frustration J', such that J' is larger than the critical value J'_c=0.602J, the quantum fluctuation of spins may completely melt the AFM order phase, resulting in the disordered SL state. However, the J'_c is unphysically large since *ab initio* calculations [13] indicate that the physical value for J'_c is $J'_c < 0.05J$. Therefore the mean-field theoretical critical value J'_c is very much larger than the real one; we believe that a smaller value of J'/J to melt the AFM order can be obtained by going beyond mean-field theory. Away from half filling, the AFM spiral order may be destroyed by both quantum fluctuation of spins and doping, and the superconductivity appears [8]. Figure 2 shows that the RVB order parameter D is almost invariant with increasing J'/J at half filling. This result is not surprising, and means that the fluctuation of spins does not destroy the RVB spin order, and favour the RVB-like SL state. On the other hand the RVB spin order can be destroyed quickly [11, 14] due to doping. Figure 3 shows that the order parameter B decreases slowly with increasing J'/J (however, $J'B/J$ increases slowly with increasing J'/J). All these results indicate that the strong quantum fluctuation may generate the SL ground state with no long-range order [2]. The relationship between doping and antiferromagnetism is a central issue in the copper oxide superconductors [4, 5]. Several studies have suggested a possible connection between pure spin systems and doped ones. It has been proposed [15] that the same effects of doping can be described by including the frustration term J' in the Heisenberg model. Our results seem to favour these ideas.

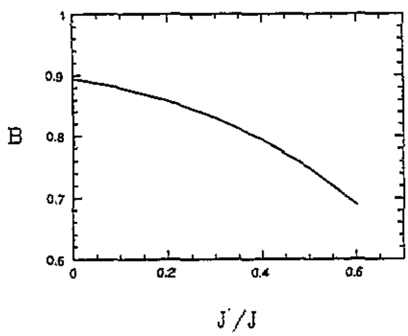

Figure 3. Variation of the order parameter B with J'/J at half filling.

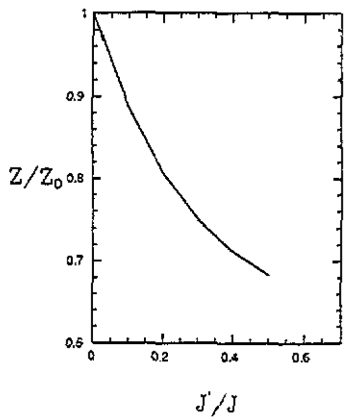

Figure 4. Variation of the linear term of the free energy Z (in units of J) with J'/J for $t/J = 4$, where $Z_0 = 2.41J$ is the value of Z at $J' = 0$.

For discussing the phase separation, we have performed an expansion [9, 10] for the free energy of the system F_{free} for small doping δ at a temperature $T = 0^+$

$$F_{\text{free}} = F_{\text{free}}(\delta = 0) + Z\delta + \tfrac{1}{2}\beta\delta^2. \tag{4}$$

For the case J'=0, our result corresponds to those obtained earlier [9, 10]. We note that the positive linear term (the chemical potential) Z is independent of t. We also find the compressibility β is negative for any values of t/J and J'/J in the case of spin $S = \frac{1}{2}$. Figure 4 and figure 5 show that Z and β change with J'/J. The negative compressibility β suggests [6] the possibility of the spiral or the SL state being unstable against the phase separation between a hole-rich phase and the no-hole phase, provided the free-energy function is minimized in the spiral or SL state at large doping. The positive linear term Z implies that the untwisted Néel state is metastable, and would suffer a first-order transition towards the true ground state. Figure 4 shows that Z decreases with increasing J'/J; this means the range of the phase separation is diminished, and the first-order transition is induced at a very low level of doping, which may be regarded as a disordered AFM or SL state depending on the value of J'/J. However, the absolute value of the compressibility β increases with increasing J'/J. This also favours the hole-rich phase and induces a tendency towards a much lower doping level where the free-energy function is minimized in the spiral or SL state. Figure 6 shows the free energy of the t–J–J' model as a function of the doping δ, where the range of phase instability is $0 < \delta < 0.095$ for J'/J =0, and $0 < \delta < 0.06$ for J'/J =0.3. Thus the range of phase separation is obviously diminished due to the quantum fluctuation of spins. According to the above discussions, the frustration term J', which describes the quantum fluctuation of spins in the mean-field approximation, seems to favour diminishing the range of the phase separation, at least in the doping range of interest for the study of the copper oxide superconductors.

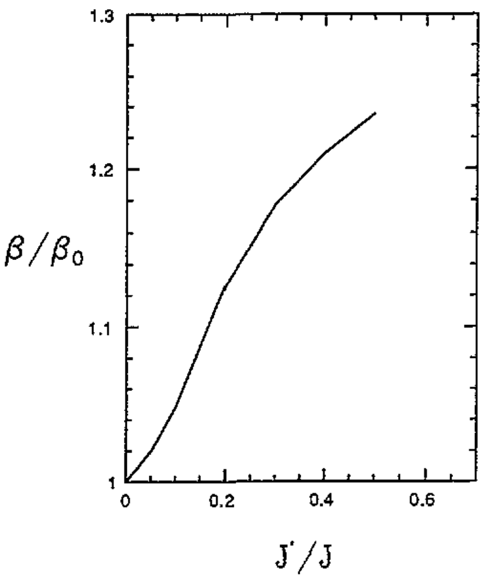

Figure 5. Variation of the compressibility β (in units of J) with J'/J for $t/J = 4$, where $\beta_0 = -48.69J$ is the value of β at $J' = 0$.

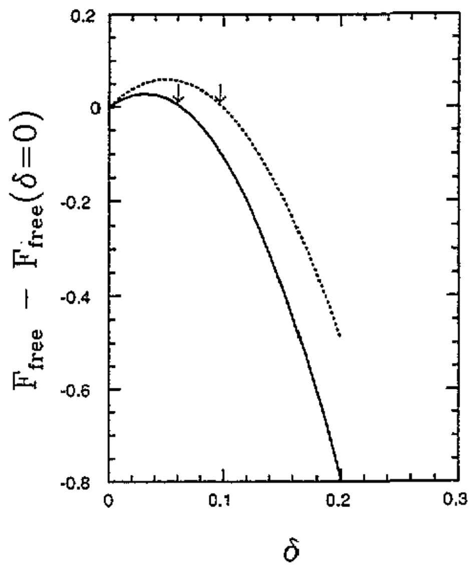

Figure 6. Free energy of the t–J–J' model as a function of doping δ for $t/J = 4$, $J'/J = 0$ (the dashed line), and $J'/J = 0.3$ (the solid line). The critical points of phase instability are indicated by arrows. The ranges of phase instability are $0 < \delta < 0.095$ for J'/J =0, and $0 < \delta < 0.06$ for J'/J =0.3.

In conclusion, we have studied the properties of the ground state and the phase instability of the t–J–J' model, which may be relevant to the study of the copper oxide superconductors, by using the Schwinger boson mean-field theory. Our results indicate that the frustration term J', which describes the quantum fluctuation of spins in the mean-field approximation, favours the RVB-like SL state and induces a tendency to diminish the range of the phase separation.

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