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Spiral phases and time-reversal-violating resonating-valence-bond states of doped antiferromagnets

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The phase diagram of the t-t'-J model is investigated with use of a slave-fermion mean-field approach. States with spiral antiferromagnetic order are found to be stable for small t/J and hole concentration δ. For larger t/J and δ, corresponding more closely to the physical parameter values of the oxide superconductor, a flux phase exhibiting a uniform chiral order is found to be more stable than the spiral states. This state breaks parity and time-reversal symmetry.

The normal state of the high-temperature oxide superconductors exhibits a number of anomalous properties which suggest that it is not an ordinary Fermi liquid.[1] In view of the fact that undoped La_2CuO_4 is an antiferromagnetic insulator, it is of considerable interest to understand how the ground state evolves as a function of doping.

Much of the theoretical effort has focussed on the large-U Hubbard model or the t-J model.[2] Two different mean-field approaches have evolved, and the connection between these two mean-field approaches has been discussed in the context of the Heisenberg model at half-filling.[3] In the slave-boson mean-field approach, the ground state for large doping is a uniform resonating-valence-bond (RVB) state with a spinon Fermi surface obeying Luttinger's theorem.[4] The low-temperature phase where the holes Bose condense is a strongly correlated Fermi liquid with antiferromagnetic correlations. Close to half-filling, the stable state of this mean-field theory is the $s+id$ or flux phase with point Fermi surfaces.[5] The slave-fermion approach, on the other hand naturally gives an ordered Neél state at half-filling,[6] which evolves into spiral antiferromagnetic states at small doping.[7] At larger doping and for moderate t/J, a ferromagnetic phase with the physics of the Nagaoka state was found.[7]

In this paper, we numerically investigate the phase diagram of the t-t'-J model[8] in the slave fermion formalism, and show that at large δ (doping parameter) and t a new RVB state is favored over both the spiral phases and the ferromagnetic states. This state has a nonzero flux in a sense to be defined below and has a uniform chiral order parameter and consequently violates parity and time-reversal symmetries. There seems to be an exact parallel between the slave-fermion and slave-boson approaches in that a state with no flux in one corresponds to a state with flux in the other.

The t-t'-J model is a generalization of the t-J model of a doped antiferromagnet constrained to the subspace with no double occupancy.

$$\begin{aligned}\mathcal{H} = &\sum f_i f_j^\dagger b_{i\sigma}^\dagger b_{j\sigma} \\ &+\frac{J}{4}\sum b_{i\alpha}^\dagger b_{i\beta} b_{j\gamma}^\dagger b_{j\delta}(\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta}-\delta_{\alpha\beta}\delta_{\gamma\delta}) \\ &+\sum\lambda_i(b_{i\sigma}^\dagger b_{i\sigma}+f_i^\dagger f_i-2s)\,, \end{aligned}\tag{1}$$

where the electron operators $c_{i\sigma}$ have been written as $c_{i\sigma}=f_i^\dagger b_{i\sigma}$ with use of slave fermions to enforce the no-double-occupancy constraint.[7,8] It is known, from studies of a hole hopping in a quantum antiferromagnet, that quantum fluctuations allow a hole to hop coherently on the same sublattice in a Neél state.[9] The t-t'-J model is a renormalized model which takes into account this same sublattice hopping process by including a term $\sum t'_{ij}c_{i\sigma}^\dagger c_{j\sigma}$.[8] The slave-fermion mean-field theory of this model has been described in detail in Ref. 8. In that work the mean-field phase diagram of this model was investigated in the region of small doping, by performing an expansion in δ, and it was shown that the ground state is a spiral antiferromagnet.[8] Here we present a numerical calculation of the complete phase diagram. The order parameters of the mean-field theory are

$$\begin{aligned} D_\eta &= \langle b_{i\uparrow}^A b_{i+\eta\downarrow}^B - b_{i\downarrow}^A b_{i+\eta\uparrow}^B\rangle\,, \\ Q_\eta &= \langle b_{i\uparrow}^{\dagger A} b_{i+\eta\uparrow}^B + b_{i\downarrow}^{\dagger A} b_{i+\eta\downarrow}^B\rangle\,, \\ F_\eta &= \langle f_i^{\dagger A} f_{i+\eta}^B\rangle\,. \end{aligned}$$

The order parameters are taken to be translationally invariant. The various states considered away from half-filling are listed in Table I. We first consider states with $D_\eta=D$, which is known to be the global minimum of this mean-field theory at half-filling.[6] Different physical states away from half-filling can be distinguished by the

TABLE I. List of the symmetries of the various states that were investigated. The last two were always found to be higher in energy than the flux state.

	D_x	D_y	$D_\eta/D_{-\eta}$	Q_x	Q_y	$Q_\eta/Q_{-\eta}$
Canted	D	D	1	Q	Q	1
Spiral (1,1)	D	D	1	Q	Q	-1
Spiral (1,0)	D	D	1	Q	0	-1
Double spiral	D	D	1	Q	iQ	-1
Flux	D	iD	1	Q	Q	-1
	D	iD	1	Q	iQ	-1
	D	iD	1	Q	iQ	1

gauge-invariant quantities $P_{\hat{\eta},\hat{\eta}'} \equiv D^*_{\hat{\eta}} Q_{\hat{\eta}} D_{\hat{\eta}'} Q^*_{\hat{\eta}'}$. The different spiral states are distinguished by $P_{\hat{x},\hat{y}}$.[8] The spiral (1,1) has Q_η with p_x+p_y symmetry and $P_{\hat{x},\hat{y}} = P_{\hat{x},\hat{x}} = P_{\hat{y},\hat{y}}$; the spiral (1,0) has Q_η with p_x symmetry and $P_{\hat{x},\hat{y}} = 0$ and the interesting double-spiral state has Q_η with $p_x + ip_y$ symmetry and $P_{\hat{x},\hat{y}} = iP_{\hat{x},\hat{x}} = iP_{\hat{y},\hat{y}}$. The phase diagram is obtained by minimizing the free energy with respect to the order parameters. We work at a small but finite temperature where there is an exponentially small gap and the condensate characterizing long-range antiferromagnetic order[6,7] does not appear. One still has to be careful in dealing with the k-space regions where the gap is exponentially small.

The phase diagram in the t-t'-J space for the states having uniform D_η with s symmetry are shown in Fig. 1. At $t'=0$, the spiral (1,1) state appears infinitesimally away from half-filling and remains the ground state until a ferromagnetic phase with $Q_\eta \neq 0$ but $D_\eta = 0$ comes in at large δ and t.[7] For larger t' and small δ, the (1,0) spiral is more stable than the (1,1) and finally for large enough t' the Neél state becomes most stable. The double spiral is never the global minimum, even though it is very close in energy where the (1,0) state is stable. This is in agreement with the analytical results of Ref. 8, which were obtained in the small δ limit. For larger δ and t, the numerical calculations show that the system goes directly from the (1,1) spiral to the Neél state without any intervening (1,0) state. The energies of the (1,1) and (1,0) are very close in this region. In Fig. 2 we show the dependence of D and Q on δ for $t/J=5$ and two different values of t'. It is clear that a finite t' inhibits the growth of the spiral order parameter Q.

The most interesting numerical results appeared when we looked at the large doping region and included in our investigation the flux states of Table I.

The bandwidth of the holes is expected to be $Qt \simeq \delta t$ in the large δ regime $\delta t > J$; this will dominate the bandwidth $\simeq J$ of a single-hole hopping in a Neél background. For this reason the t-t'-J model is not very meaningful, and we therefore looked at the pure t-J model in this region. At half-filling, where only $D_\eta \neq 0$, there are two saddle-points of the mean-field equations: (i) the uniform phase with $D_\eta = D$ and (ii) the flux phase ($s+id$ phase of Ref. 6) with $D_y = iD_x$. The flux phase is higher in energy at half-filling. It also has a very different condensate wave function. It is known that in the uniform phase a condensate appears for spin $S>0.19$ which signifies long-ranged Neél order. This condensate is described by $\langle b^{A}_{(m,n)\uparrow}\rangle = \sqrt{n_0}$, $\langle b^{B}_{(m,n)\downarrow}\rangle = \sqrt{n_0}$ which gives a spin-up–spin-down ordering, and corresponds to the gap going to zero at $\mathbf{k}=(0,0)$ in our reduced Brillouin zone [which is shifted by $(\pi/2,\pi/2)$ from the original Brillouin zone]. A condensate also appears in the flux phase but only for $S>0.4$, and in this case the gap goes to zero at $\mathbf{k}=(0,0)$ and $(0,\pi)$. In the flux state the condensate can be described only by going to a doubled real-space unit cell. The order parameter D is, however, defined within the smaller unit cell and there are no solutions to the mean-field equations which are consistent with the chosen symmetry of D and the condensate. Our attitude at this point is to treat the flux phase as a state with a finite gap, since it would be so even for a static distribution of 20% holes which brings S

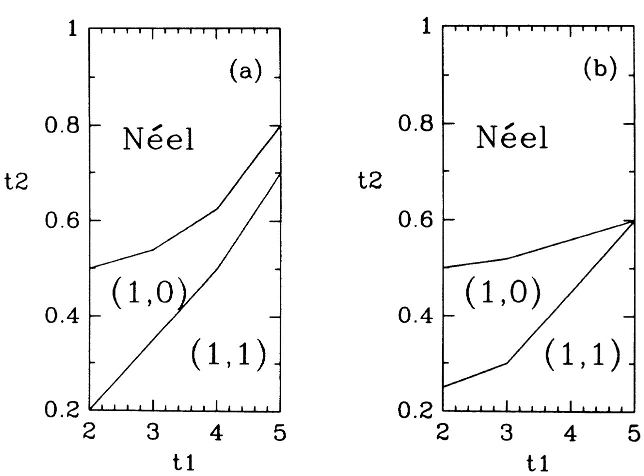

FIG. 1. Phase diagram of the t-t'-J model in the t-t' plane ($t1 \equiv t/J$), $t2 \equiv t'/J$), in the space of uniform D_η states (a) for $\delta=0.05$, (b) for $\delta=0.10$.

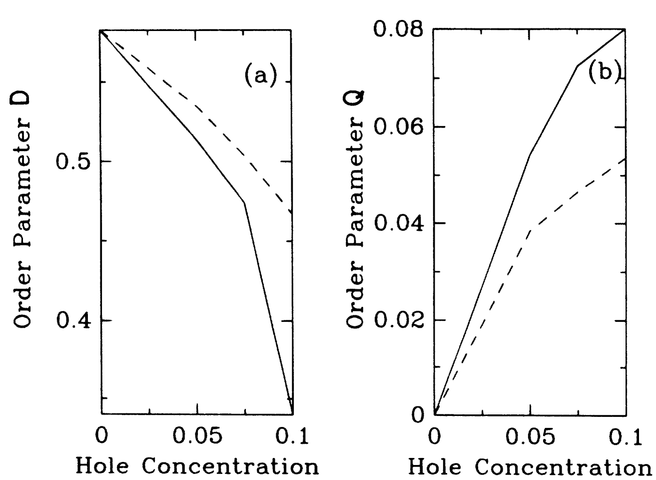

FIG. 2. Variation of the order parameters D and Q with the hole concentration δ. (a) shows variation in D for $t2=0$ (solid line) and $t2=0.5$ (dashed line). (b) shows variation of Q for the same two values of $t2$.

down to 0.4. For a finite hopping amplitude t, and a nonzero value of Q_η, this is expected to occur for even smaller δ. A study of the temperature dependence of the correlation length also shows a much more dramatic decrease with increasing temperature for the flux phase than the uniform phase.

The disordered flux state, with no condensate, at half-filling can be described by a variational wave function[8]

$$|\Psi\rangle \alpha \exp\left[\sum_k \frac{D_k}{|D_k|} b^{A\dagger}_{-k\uparrow} b^{B\dagger}_{-k\downarrow} - \frac{D_k^*}{|D_k|} b^{A\dagger}_{k\downarrow} b^{B\dagger}_{-k\uparrow}\right]|0\rangle .$$

When projected onto the constrained subspace this becomes a finite-range RVB wave function[10] with singlets between sites on opposite sublattices and with a phase $e^{i\theta}$ associated with these singlets, where θ is the angle the bond makes with the x axis. This is in contrast to the s-wave state $D_\eta = D$ where there are no phases associated with the singlets.

Away from half-filling we investigate a state with flux in D_η, and a Q_η with $p_x + p_y$ symmetry (the other states listed in Table I are higher in energy), such that

$$P_{\hat{x},\hat{y}} \equiv D_x^* Q_x D_y Q_y^* = i|D|^2|Q|^2 = iP_{\hat{\eta},\hat{\eta}} ,$$
$$P_{\hat{\eta},\hat{\eta}} = -P_{\hat{\eta},\hat{\eta}} . \quad (2)$$

This is a state with a *uniform* chiral order parameter $[\mathrm{Im}P_{\hat{x},\hat{y}} = 4S\langle \mathbf{S}_i^A \cdot (\mathbf{S}_{i+x}^B \times \mathbf{S}_{i+y}^B)\rangle]$,[8,11] in contrast to the double-spiral state obtained with s-wave D_η,[8] which has a staggered chiral order parameter. This follows from the observation that D_n transforms to $-D_\eta$ and Q_η transforms to Q_η^* on changing the sublattice. This flux state would therefore seem to be disordered for any finite Q since it is difficult to reconcile condensation with a nonzero chiral order parameter.[8] The spinon dispersion in this flux state is

$$\omega_k^{\pm} = [(\mu \pm |M_k|)^2 - |\tfrac{1}{2} J D_k|^2]^{1/2}$$

with

$$D_k = 2D(\cos k_x + i \cos k_y)$$

and

$$M_k = (\tfrac{1}{2} JQ + 2tF)(\sin k_x + \sin k_y) .$$

The minima in the dispersion occur at (0,0) and $(0,\pi)$ and its permutations when $Q=0$ and shifts to (k_0,k_0) and $(k_0,\pi-k_0)$ with increasing Q, where k_0 is proportional to Q. This state therefore has point zeroes unlike the double-spiral state which has a ring of zeroes. Viewed in terms of a wave function for spins, a phase $e^{i\theta}$ (proportional to the bond angle) appears in the same sublattice singlets in the double spiral, whereas they appear in the opposite sublattice singlets in the flux phase.

In our numerical investigation, we found that the flux phase becomes stable when t and δ are beyond a critical value. The phase boundary between the spiral (1,1) and the flux phase is shown in Fig. 3. It is interesting to compare this to the phase diagram obtained in the slave-boson picture where the no-flux phase appears in the same region where we find a flux phase. In this region of the t-δ phase space the order parameters D and Q are nearly equal and smaller than $2tF$, which therefore dominates the spinor dispersion relation. The minima of the spinon dispersion shift to $k \simeq (\pi/2,\pi/2)$ in the reduced Brillouin zone.

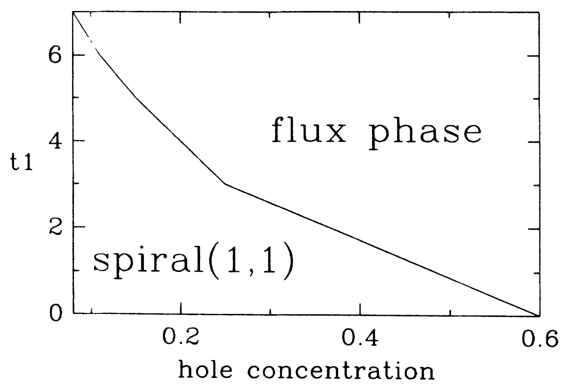

FIG. 3. Phase diagram in the t-δ plane showing the region of stability of the flux phase (see text). The phase is seen to be stable in the region of interest to high-temperature superconductivity.

The region of stability of the flux phase is precisely the region of interest in the study of the oxide superconductors ($t/J \sim 5$, $\delta \simeq 0.1$).

The occurrence of a phase with a *uniform* chiral order parameter and a flux in $b^\dagger b$ in the region of physical parameter values is extremely intriguing. The phases associated with the valence bonds allows for the possibility of a transmutation of the statistics of the elementary excitations, the spinons and holons.[12,13] As discussed in Ref. 12, the nominal statistics of the excitations can be altered by the binding of vortices, and under certain circumstances this process lowers the energy of the excitations. Such an effect might produce a state more like a Fermi liquid as in the slave-boson approach.[4] Alternatively, the existence of a nonvanishing chiral order parameter could lead to the appearance of excitations with fractional statistics[13] These possibilities are currently being investigated.

In conclusion, we have mapped out the phase diagram of the t-t'-J model and shown that same sublattice hopping favors the Neél state. More importantly we have shown that in the region of interest to the high-temperature superconductors, a state with a uniform chiral order parameter and no long-range spin order, becomes more stable than the incommensurate spiral antiferromagnetic states found at small δ. The appearance of this flux phase eliminated the large ferromagnetic region of the phase diagram.

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