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LETTER TO THE EDITOR

Staggered flux phase and d-wave phase of the *t–J* model

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Abstract. We have numerically evaluated the energy of the staggered flux phase state (SFP), the d-wave resonating valence bond state, and the mixed SFP and d-wave state (SFP + d) of the extended *t–J* model at various hole densities (δ). The flux per plaquette and the size of the d-wave gap are taken as variational parameters. The calculation includes the kinetic energy, spin energy, the effective hole–hole interaction and the three-site pair-hopping term. We found that the SFP is stable against the projected Fermi liquid up to $\delta \simeq 20\%$.

For moderately large J, $J/t \geq 0.4$, the SFP + d state may be favoured against the pure d-wave state but only at very low hole density ($\delta \sim 2\%$). These calculations show that the pure SFP state is never the ground state at hole densities of experimental interest.

One of the most interesting and exotic possibilities for the ground state of the two-dimensional *t–J* model is the staggered flux phase (SFP) state. This was first proposed by Affleck and Marston [1] on the basis of a large-N expansion, where N is the number of fermion flavours. Variationally, this state corresponds to putting non-interacting electrons into the ground state of a system the lattice of which is pierced by magnetic flux lines whose directions alternate in a checkerboard pattern. This is followed by Gutzwiller projection. Two interesting questions arise: first, whether this can even be the ground state of the model; second, what is the relation, if any, to superconductivity. One of us recently discussed these issues within a mean-field theory [2], computing the energies of the SFP state and a mixed SFP and d-wave superconducting (SFP + d) state. The d-wave pairing state considered has a Cooper pair wavefunction of Γ_3 symmetry, i.e., $\Delta(k)$ is proportional to $\cos k_x a - \cos k_y a$, where k is the momentum and a is the lattice constant. The coexistence state may be constructed in various ways. We give our prescription below (see equations (2) and (3)). The mean field approximation suggests that there is a region of stability in parameter space for the SFP + d state in the presence of the hole–hole interaction. This motivated us to use the variational Monte Carlo method to carry out the calculation within the space of Gutzwiller wavefunctions. The constraint that no sites are doubly occupied is obeyed exactly in this method.

We search the parameter space of v_{nn} (nearest neighbour hole–hole interaction) over a wide range, δ (hole density) from 0–20% hole concentration, and φ (flux per plaquette) $= n/10$ (with $n = 0, 1, \ldots, 5$). We compare the energies of the SFP state, the SFP + d state, the pure d-wave state and the Fermi liquid (FL) state. All our simulations were performed on an 82 site lattice.

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The Hamiltonian we use is defined as follows

$$H = T + H_2 + H_3 + H_4 \qquad T = -t \sum_{\langle ij\rangle,\sigma} (a^\dagger_{i\sigma} a_{j\sigma} + \text{HC})$$
$$H_2 = J \sum_{\langle i,j\rangle} (S_i \cdot S_j - n_i n_j/4)$$
$$H_3 = -\tfrac{1}{4} J \sum (a^\dagger_{i+j\sigma} a_{i-\sigma} a^\dagger_{i-\sigma} a_{i+k\sigma} - a^\dagger_{i+j-\sigma} a^\dagger_{i\sigma} a_{i\sigma} a_{i+k\sigma}) \tag{1}$$
$$H_4 = v_{nn} \sum_{\langle i,j\rangle} (1 - n_i)(1 - n_j).$$

In these formulae $a^\dagger_{i\sigma} = (1 - n_{i\bar{\sigma}}) c^\dagger_{i\sigma}$ where $c^\dagger_{i\sigma}$ is the electron creation operator. $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and $n_i = \Sigma_\sigma n_{i\sigma}$. In H_3, the three-site term, the sum runs over nearest neighbours j and k of site i, which are such that $j \neq k$. The three-site term is often ignored because of its complexity but at high hole concentration its expectation value can be comparable to H_2, the Heisenberg term. H_4 is the effective hole–hole interaction on neighbouring sites. The wavefunctions we use may be written as follows,

$$|\varphi\rangle = P_N P_D \prod_k (u_k + v_k \tilde{c}^\dagger_{k\uparrow} \tilde{c}^\dagger_{-k\downarrow}) |0\rangle. \tag{2}$$

In this formula P_N is the projection on to the N particle subspace and P_D is the usual Gutzwiller projection onto the subspace of no doubly occupied sites.

We define $\tilde{c}_{k\sigma} = \alpha_k c_{k\sigma} + i\beta_k c_{k+Q\sigma}$ where $\alpha_k = [(E_k + \gamma_+ \cos\theta)/2E_k]^{1/2}$, $\beta_k = [(E_k - \gamma_+ \cos\theta)/2E_k]^{1/2} \operatorname{sgn}(\gamma_-)$ when k belongs to the first half Brillouin zone ($\frac{1}{2}$BZ) (i.e. $(\cos k_x + \cos k_y) > 0$). For k outside this region, $\alpha_k = \alpha_{k-Q}$ and $\beta_k = \beta_{k-Q}$. $\gamma_\pm = 2t(\cos k_x \pm \cos k_y)$ and $\operatorname{sgn}(\gamma_\pm) = +1$ if $\gamma_\pm \geqslant 0$, $\operatorname{sgn}(\gamma_\pm) = -1$ if $\gamma_\pm < 0$. $E_k = [(\gamma_+ \cos\theta)^2 + (\gamma_- \sin\theta)^2]^{1/2}$ and the energy of the electron state is $-E_k \operatorname{sgn}(\gamma_+)$. $4\theta/2\pi = \Phi$ is the expression for the flux per plaquette and $Q = (\pi, \pi)$. We set

$$v_k/u_k = \Delta_k / \{-E_k \operatorname{sgn}(\gamma_+) - \mu_0 + [\Delta_k^2 + (-E_k \operatorname{sgn}(\gamma_+) - \mu_0)^2]^{1/2}\} \tag{3}$$

where $\Delta_k = \Delta_d \gamma_-/t$ is related to the superconducting order parameter, and μ_0 is the Fermi energy.

From the expression for the trial wavefunction, we can see that if we set $\theta = 0$ (i.e. no flux state) then we would have $\beta_k = 0$ and $\alpha_k = 1$, and (2) will be reduced to the usual expression for the projected BCS wavefunction. However, if we have $u_k = 0$, $v_k = 1$ when k belongs to the first half Brillouin zone and $u_k = 1$, $v_k = 0$ when k does not belong to the zone then (2) will reduce to the eigenstates of free electrons in the presence of a staggered flux.

Thus, in our calculation, we have two variational parameters: Φ(flux) and Δ_d (order parameter). The energy is minimized with respect to these parameters to find the ground state. There are different stable states corresponding to different physical parameters δ, v_{nn} and J/t. $\Delta_d = 0$, $\theta \neq 0$ corresponds to a pure staggered flux phase state; $\theta = 0$, $\Delta_d \neq 0$ is a pure superconducting d-wave RVB state (if $\delta > 0$); $\theta \neq 0$, $\Delta_d \neq 0$ is a mixed SFP and superconducting state. Finally $\theta = 0$, $\Delta_d = 0$ is simply the projected Fermi liquid state. In general, the wavefunction represents a state in which the SFP and the superconducting state coexist.

The algorithm used has been described in general terms previously [3]. We verified that the present version reproduced earlier results. In particular, the trial wavefunction

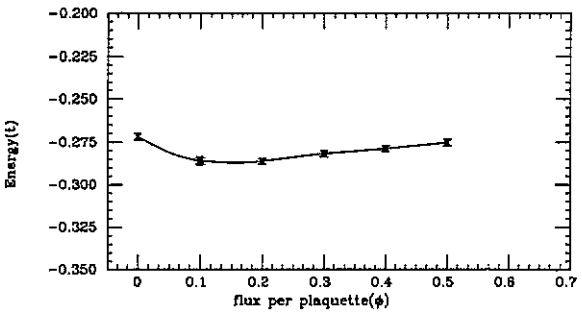

Figure 1. Total energy as a function of φ, the variational parameter for the staggered flux phase state at fixed $\delta(= 2.4\%)$ and $J/t = 0.4$. The simulations were performed on an 82 site lattice with 6×10^4 Monte Carlo steps.

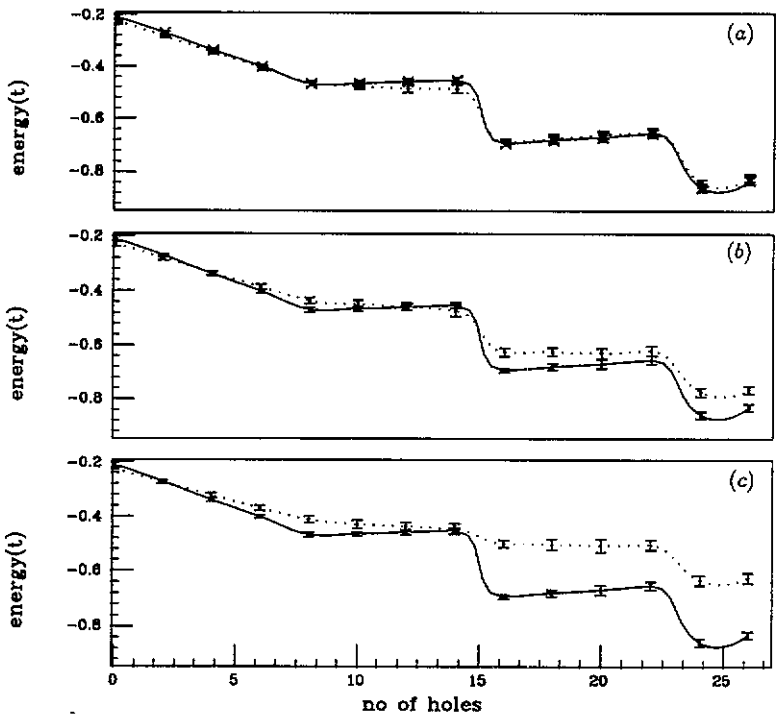

Figure 2. Total energy as a function of holes of the SFP state ($\cdots$) and the FL state (——) at $J/t = 0.4$ and $\Delta_d = 0$, with (*a*) $\Phi = \frac{1}{10}$ (*b*) $\Phi = \frac{2}{10}$ (*c*) $\Phi = \frac{3}{10}$.

produces exactly the same energy as that from the previous d-wave RVB [4] results when we set $\theta = 0$ and $\Delta_d \neq 0$.

To indicate how the stability of the various states was established, we give some results from typical runs. For simplicity $v_{nn} = 0$ initially. In figure 1, we show the energy versus flux at a fixed doping level $\delta = 2.4\%$, and a fixed value of $J/t = 0.4$. In figure 2, we show the comparison of three different SFP states and the FL state as a function of doping. From the figure it can be seen that the SFP is stable against the projected Fermi liquid up to $\delta = 20\%$. This is qualitatively consistent with the mean field results of [1], though the parameters there should be renormalized. The oscillations are due to the filling of shells in momentum space, an effect always present in a finite size calculation. The oscillations introduce some error in the phase boundaries as a function of δ.

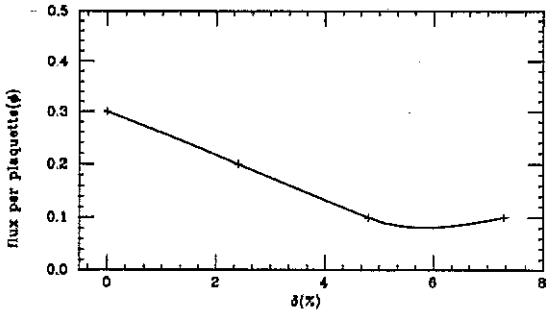

Figure 3. The flux (φ) of the favourable state versus δ, the hole density. At each hole doping, we search the flux space to find the lowest energy state.

One of our main results is shown in figure 3, which gives the most favourable flux value as a function of doping. There are several interesting aspects to this plot. At half filling ($\delta = 0$), the Hamiltonian (1) reduces to the antiferromagnetic Heisenberg model. It is invariant under the local SU(2) transformation [5, 6]:

$$c_{i\uparrow} \rightarrow \alpha_i c_{i\uparrow} + \beta_i c_{i\downarrow}^{\dagger} \qquad c_{i\downarrow}^{\dagger} \rightarrow -\beta_i^{*} c_{i\uparrow} + \alpha_i^{*} c_{i\downarrow}^{\dagger}$$

where $|\alpha_i|^2 + |\beta_i|^2 = 1$. A SFP state with flux φ is transformed to a d-wave state with parameter Δ_d if $\tan(\pi\varphi/2) = \Delta_d/t$. The commensurate uniform flux phase (flux equal to half a flux quantum per plaquette) is equivalent to the SFP with $\varphi = \frac{1}{2}$. This is the ground state in the mean-field theory. Our results at half filling show that this is *not* true when the projection is treated exactly. In fact a SFP state with $\varphi = 0.3$ is lowest in energy, showing that the uniform flux phase is not stable with respect to the SFP. More general wavefunctions with additional phase factors for the holes in the commensurate uniform flux state have been introduced by Ogata *et al* [7]. As these authors show, the energy is not changed too much when this is done. Thus we also expect that these more sophisticated states will also be unstable with respect to the SFP. Note also that extensive investigations of Nori *et al* [8] have shown that the state with precisely one flux quantum per electron per spin is always the lowest in energy. Hence it is unlikely that other field strengths need to be examined for comparison purposes. These results are consistent with earlier calculations in the pure d-wave state [3, 4] which showed that $\Delta_d = 0.5t$ is lower in energy than the mean-field solution $\Delta_d = t$.

This numerical calculation therefore demonstrates that the commensurate flux phase (CFP) is locally unstable to fluctuations in the flux of rather short wavelength. This casts some doubt on the relevance of the numerous discussions of the excitations of the CFP (particularly having to do with their statistics). The mean-field theory results on this phase may actually be investigations of the neighbourhood of a saddle point, and not a minimum, of the energy.

Table 1. Comparison of the total energy E per site, kinetic energy E_{kin} per hole and spin energy $JS_i \cdot S_j$ of the optimal SFP state with and without the presence of a small superconducting order parameter. $J/t = 0.4$. All energies are in units of t.

	$\delta = 2.44\%$			$\delta = 4.88\%$		
	E	E_{kin}	$JS_i \cdot S_j$	E	E_{kin}	$JS_i \cdot S_j$
$\Delta_d = 0$	−0.286(1)	−2.67(3)	−0.282(1)	−0.347(2)	−2.65(2)	−0.249(1)
$\Delta_d = 0.1t$	−0.288(1)	−2.65(1)	−0.286(1)	−0.350(1)	−2.63(1)	−0.260(1)

Table 2. Comparison of the total energy E per site, kinetic energy E_{kin} per hole and spin energy $JS_i \cdot S_j$ of the optimal d-wave state with and without the presence of a small amount of staggered flux. $J/t = 0.4$. All energies are in terms of t.

	$\delta = 2.44\%$			$\delta = 4.88\%$		
	E	E_{kin}	$JS_i \cdot S_j$	E	E_{kin}	$JS_i \cdot S_j$
$\varphi = 0$	−0.290(2)	−2.64(4)	−0.293(1)	−0.352(1)	−2.60(1)	−0.272(1)
$\varphi = 0.1$	−0.290(2)	−2.61(3)	−0.295(2)	−0.351(1)	−2.56(2)	−0.275(1)

When holes are introduced, the flux goes down rapidly. Indeed, for $\delta > 5\%$, the preferred state is always the one with the smallest flux per plaquette, i.e., $\varphi = 0.1$.

In order to understand whether superconductivity can occur in this picture, we studied whether the SFP state was locally stable against d-wave superconductivity and vice versa. Initially, we set $v_{nn} = 0$. The results are summarized in tables 1 and 2. It is clear that the SFP is always unstable to d-wave pairing, and is therefore never even a local minimum. In contrast, the d-wave state is always stable against the introduction of staggered flux. These results are consistent with the renormalized mean-field theory [2].

One may also check global stability for selected cases. We verified that the SFP state at the optimal flux values was always higher in energy than the mixed (SFP + d) state with the same flux and $\Delta_d = 0.5t$. Given this, it is natural to compare the SFP + d state with the pure d-wave state, both with $\Delta_d = 0.5t$. Typical results are shown in figure 4(*a*). The d-wave state is consistently lower in energy, though the energy difference for low doping levels is small.

The addition of the long-range Coulomb interaction could help to stabilize the SFP.

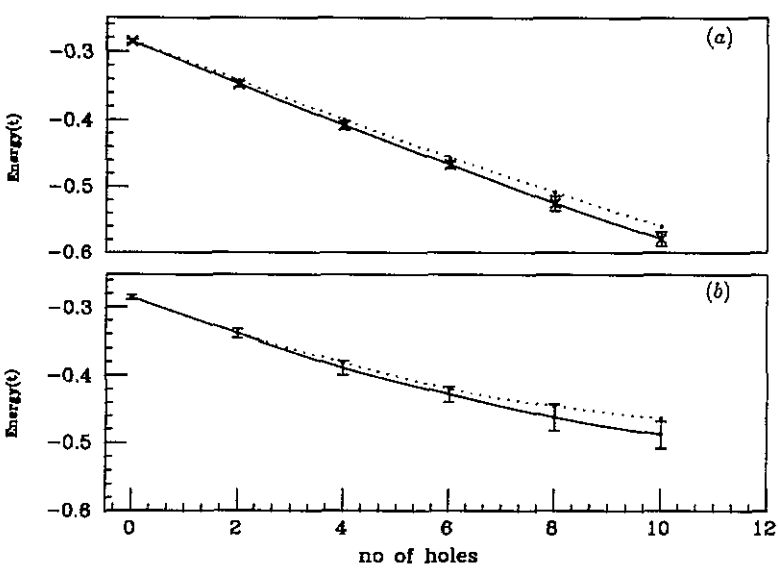

Figure 4. Total energy as a function of hole density for the SFP + d state (· · ·) and the d-wave RVB (——) state at $J/t = 0.5$ and $\Delta_d = 0.5t$: (*a*) without the H_4 term ($v_{nn} = 0$); (*b*) with the H_4 term ($v_{nn} = 6.4t$).

Table 3. Hole–hole correlation function g_1, as defined in the text, for various states. The statistical error is about 20% when $\delta < 7\%$ and is about 10% when $\delta > 7\%$.

δ(%)	FL	SFP	d wave	SFP + d($\Phi = 0.1$)	SFP + d($\Phi = 0.2$)
2.44	0.00023	0.00021	0.0012	0.00099	0.00058
4.88	0.0015	0.0013	0.0030	0.0029	0.0030
7.32	0.0032	0.0033	0.0062	0.0065	0.0057
9.76	0.0062	0.0061	0.0098	0.010	0.0099
12.2	0.013	0.012	0.014	0.015	0.015

Accordingly, we calculated the hole–hole correlation function f_1 for several states, where

$$g_1 = \frac{1}{L}\sum_{\langle ij\rangle}(1-n_i)(1-n_j)$$

where L is the number of sites. The results are shown in table 3. We may state generally that

$$g_1(\text{d-wave}) \approx g_1(\text{FL}) > g_1(\text{SFP})$$

in an obvious notation. Therefore a positive v_{nn} favours the SFP. However, the differences are sufficiently small that there is little effect on the overall stability question. In figure 4(b), we compare the SFP + d and d-wave states for $v_{nn} = 6.4t$ (a rather large value) and find that the energy difference is narrowed but does not change sign except perhaps for $\delta < 2\%$. The general conclusion for a very wide range of v_{nn} and δ is that the hole–hole interaction is not important.

Since we have done a thorough calculation in a wide range of parameter space including the three-site term and the hole–hole effective interaction, we can conclude that the SFP + d state is not a candidate for the t–J model for J/t smaller than 0.5 except at very small doping. At these low hole concentrations, high T_c materials are insulating.

After completion of our calculation we received a preprint by Lee and Chang. Some of their results, in particular on the pure SFP, are consistent with the above. Also, a paper [9] appeared which showed that a superconducting phase with a staggered flux structure is stable at large N. Our results show that this is probably not the case at $N = 2$.

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