RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 42, NUMBER 4 1 AUGUST 1990

Phases of the t-J model from variational Monte Carlo studies: Occurrence of time-reversal symmetry breaking

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(Received 17 May 1990)

We have numerically evaluated the energy of several kinds of wave functions considered to be candidate ground states of the two-dimensional t-J model at various hole densities. We searched a parameter space which includes d-wave and s-wave superconductivity and spin-density-wave ordering as well as the projected Fermi-liquid state. Coexistence of different orderings, such as the $s+id$ state and d-wave spin-density-wave state, were found to be stable states. We find a phase diagram in the density-t/J plane which has coexistence of antiferromagnetism and superconductivity at very low hole concentrations and superconductivity up to rather high values of density —about 40%. At intermediate concentrations, the time-reversal symmetry breaking $s+id$ state is found.

The strong-coupling Hubbard model was the first to be proposed as a model for high-T_c superconductivity.[1] More specifically, the one-band t-J model was shown to provide a consistent description of the low-lying energy levels of copper oxide sheets.[2] Recent first-principles calculations indicate that the parameter regime of the real materials is one in which the t-J model applies.[3]

This makes it imperative to understand the phase diagram of the model as a function of the only dimensionless energetic parameter in the model, namely J/t, and the hole density δ which can be adjusted in the experimental system by doping. $\delta=1-n$, where n is the number of electrons per site. We present here a calculation of this phase diagram within the space of Gutzwiller wave functions, defined here as Hartree-Fock or BCS one-particle wave functions which are projected on the subspace of the one-band Hilbert space in which no sites are doubly occupied. The no-double-occupancy constraint is thus satisfied exactly, in contrast to mean-field slave-boson treatments. We compare our results to those arising from other methods below.

The Hamiltonian we use is

$$H=T+H_2+H_3,$$

where

$$T=-t\sum_{\langle ij\rangle\sigma}(a_{i\sigma}^{\dagger}a_{j\sigma}+\text{H.c.}),$$

$$H_2=J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-n_in_j/4),$$

$$H_3=-\tfrac{1}{4}J\sum_{\substack{\langle ij\rangle\\\langle ik\rangle}}(a_{i+j\sigma}^{\dagger}a_{i-\sigma}^{\dagger}a_{i-\sigma}a_{i+k\sigma}-a_{i+j-\sigma}^{\dagger}a_{i\sigma}^{\dagger}a_{i-\sigma}a_{i+k\sigma}).$$

In these formulas $a_{i\sigma}^{\dagger}=(1-n_{i-\sigma})c_{i\sigma}^{\dagger}$, where $c_{i\sigma}^{\dagger}$ is the electron creation operator, $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$, and $n_i=\sum_{\sigma}n_{i\sigma}$. In H_3, the three-site term, the sum runs over nearest neighbors j and k of site i which are such that $j\neq k$. The three-site term is often ignored because of its complexity. It has important physical effects at moderate doping levels, as we shall see below.

The wave functions we use may be written as follows:

$$|\psi\rangle=P_NP_D\prod_{\mathbf{k}}(u_{\mathbf{k}}+v_{\mathbf{k}}d_{\mathbf{k}\uparrow}^{\dagger}d_{-\mathbf{k}\downarrow}^{\dagger})|0\rangle.$$

In this formula P_N is the projection onto the N-particle subspace and P_D is the usual Gutzwiller projection onto the subspace of no-doubly-occupied sites. $v_{\mathbf{k}}/u_{\mathbf{k}}=\Delta(\mathbf{k})/\{\xi_{\mathbf{k}}+[\xi_{\mathbf{k}}^2+|\Delta(\mathbf{k})|^2]^{1/2}\}$, where $\xi_k=-2t(\cos k_x+\cos k_y)-\mu$ and μ is the Fermi energy. Thus, $v_{\mathbf{k}}$ and $u_{\mathbf{k}}$ are the usual BCS coherence factors for a momentum-dependent gap function. Furthermore, $d_{\mathbf{k}\sigma}=\alpha_{\mathbf{k}}c_{\mathbf{k}\sigma}+\sigma\beta_{\mathbf{k}}c_{\mathbf{k}+\mathbf{Q}\sigma}$ is the Hartree-Fock spin-density-wave destruction operator. We set $\mathbf{Q}=(\pi,\pi)$, appropriate for a commensurate antiferromagnet, and $\alpha_{\mathbf{k}}^2=\frac{1}{2}+\frac{1}{2}\cos\theta_{\mathbf{k}}$, $\beta_{\mathbf{k}}^2=\frac{1}{2}-\frac{1}{2}\cos\theta_{\mathbf{k}}$, with $\cos^2\theta_{\mathbf{k}}=1+\Delta_A^2/(\xi_k+\mu)^2$. These are the standard mean-field expressions and they involve the variational parameter Δ_A, which controls the sublattice magnetization. We take, in addition, a rather general expression for the superconducting-gap function:

$$\Delta(\mathbf{k})=\Delta_S(\cos k_x+\cos k_y)+\Delta_D(\cos k_x-\cos k_y),$$

which represents a mixture of extended s-wave and d-wave superconductivity. There are, therefore, three variational parameters Δ_A, Δ_S, and Δ_D which are varied at any given value of t/J and δ. The energy is minimized with respect to these parameters to find the ground state. Note that $\Delta_S=\Delta_D=0$ corresponds to a pure antiferromagnetic

state, $\Delta_A = 0$ is a pure superconductor (if $\delta > 0$), and $\Delta_A = \Delta_S = \Delta_D = 0$ is simply the projected Fermi-liquid state. In general, the wave function represents a state in which antiferromagnetism and superconductivity coexist.

The wave function we use is different from that of Lee and Feng.[4] They multiplied a projected BCS wave function by a modulation factor to represent the spin-density wave. Our wave function has the advantage of reducing to the projected Hartree-Fock antiferromagnet in the case where $\Delta_S = \Delta_D = 0$. This latter state is the one which is known to be very accurate close to half filling where the antiferromagnetism is important.

The results in the half-filled case are as follows. A pure d-wave state with $\Delta_D \cong t$ is favored in the superconductivity sector, as previously found by Gros.[5] Additional energy is gained by turning on Δ_A, as shown in Fig. 1. The equilibrium value is $\Delta_A = 0.15t$; our calculations show that this corresponds to a staggered magnetization of 0.15 in units where the Néel state has a magnetization of $\frac{1}{2}$. The ground-state energy is $(-0.3305 \pm 0.0004)J$, to be compared, for example, with $-0.331J$.[6] Of course at half filling the system is insulating, and the fact that $\Delta_D \neq 0$ does not imply the existence of a nonzero superfluid density.

Away from half filling, we find that antiferromagnetism quickly disappears, but superconductivity remains. The transition appears to be of second order, as may be seen from Fig. 2. We investigated the energy as a function of Δ_D and Δ_A in the region of small doping $\delta < 0.05$. The equilibrium value of Δ_D remains essentially constant: $\Delta_D \approx t$ while $\Delta_A \to 0$ along a line in the δ-J/t plane, shown as the lower curve in Fig. 3. This is, therefore, identified as the phase boundary between the coexistence state, stable at very small δ, and the pure superconducting state.

In the superconducting regime of intermediate hole concentrations we did a parameter search in the space of Δ_D and Δ_S, choosing Δ_D to be pure real and Δ_S to be either pure real or pure imaginary—the $s+d$ and $d+is$ states, respectively. The latter is degenerate with the $s+id$ state, so this is how we refer to it. Other possibilities may be considered but they are not stable in a simple Landau theory. Also, the computation involved is sufficiently extensive that only a restricted region of the parameter space can be investigated. We found that the $s+d$ state is always unstable. The $s+id$ state, on the other hand, is clearly stable at higher doping levels, as suggested by calculations of Kotliar.[7] These results are not too dissimilar from the mean-field results of Inui *et al.*[8] except that they found that an $s+d$ state was stable rather than an $s+id$ state. They also found a region of pure s wave, which we did not. A crucial difference is the inclusion here of the three-site term, which dominates the spin-spin term at $\delta > 20\%$.

At higher hole concentrations, we observe a transition from the superconducting to the Fermi-liquid state. These calculations are more difficult than the calculations at low hole concentrations for two reasons. The finite size pro-

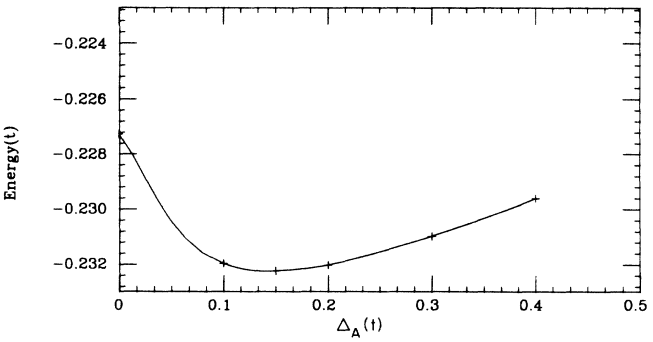

FIG. 1. Total energy in units of t as a function of Δ_A, the variational parameter for spin-density-wave ordering, in a background d-wave superconducting state. $\Delta_D = t$, $J/t = 0.4$, $\delta = 0$ is the case considered. Errors are less than 0.2%, so the minimal value of Δ_A can be located rather precisely. The simulations were performed on an 82-site lattice with 8×10^6 Monte Carlo steps.

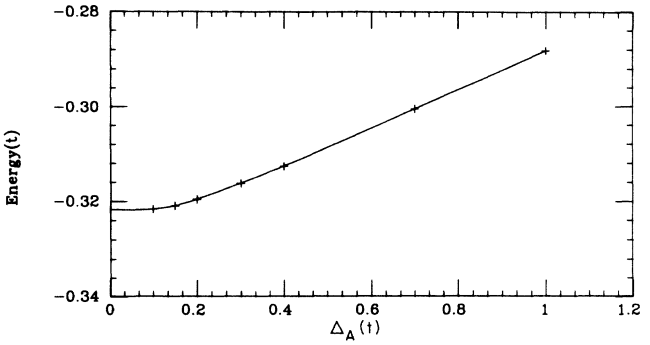

FIG. 2. Total energy in units of t as a function of Δ_A for $\delta = 0.05$. Parameters are otherwise as in Fig. 1. The minimum appears to move continuously to $\Delta_A = 0$ as a function of δ, indicating a second-order transition.

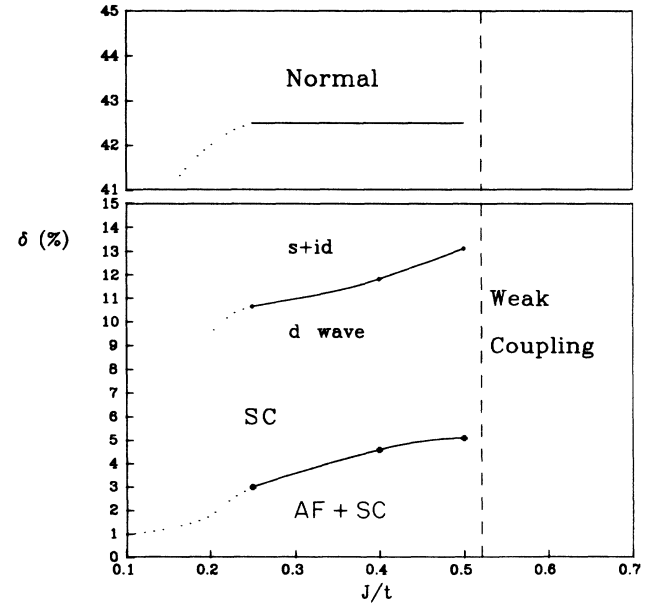

FIG. 3. Phase diagram of the model as a function of δ and J/t. High values of J/t correspond to an unphysical regime of the model and therefore they are not considered.

duces strong oscillations in the energy as a function of density due to shell effects in momentum space. Also, the three-site term is very important for $\delta \gtrsim 0.15$ and the calculation of this term is time consuming. The energy difference for a single case is plotted in Fig. 4. An average over the oscillations is given by the straight line. The phase boundary is determined by the intersection of this line with the axis. This produces the upper phase boundary in Fig. 3. Somewhat surprisingly, the superconducting state persists up to the rather high hole density of $\delta \approx 0.4$. This confirms the general idea that the Fermi-liquid state is not very stable in this model. It seems likely that this state would be unstable to some other state of higher entropy than the $s+id$ state, which would then be the actually observed normal state.

Let us now compare these results with experiments, taking $J/t \approx 0.28$[3]. The position of the lower phase boundary is in good accord with experiment,[9] but the low-density phase is insulating in the real system. In the $La_{2-x}Sr_xCuO_4$ system, in which the density is easily tuned, we expect considerable disorder due to the Sr charges. It is, therefore, reasonable to suppose that a certain number of holes would be localized in this system, an effect which does not occur in the above calculations on a perfectly homogeneous lattice. If the localization transition takes place near the magnetic transition as a function of δ, then our results are certainly consistent with the observations. We note, in particular, that no metallic phase comes between the superconducting and the antiferromagnetic phase in both theory and experiment.

We find a definite transition between a d state and an $s+id$ state as a function of doping. It is tempting to associate the former with the $T_c = 60$ K phase of $YBa_2Cu_3O_{7-\delta}$, and the latter with the $T_c = 90$ K phase. In the 90-K phase, this would be consistent with penetration-depth measurements,[10] since the $s+id$ state is completely gapped. The rather peculiar NMR results are probably also consistent with such a state.[11] The $s+id$ state breaks time-reversal symmetry. It is not clear, however, that it would generate internal magnetic fields, because the gradient terms in the free energy have an unusual form.[12] At present, we do not know if this state is consistent with recent μSR results.[13] It would be consistent with the observation of circular dichroism.[14]

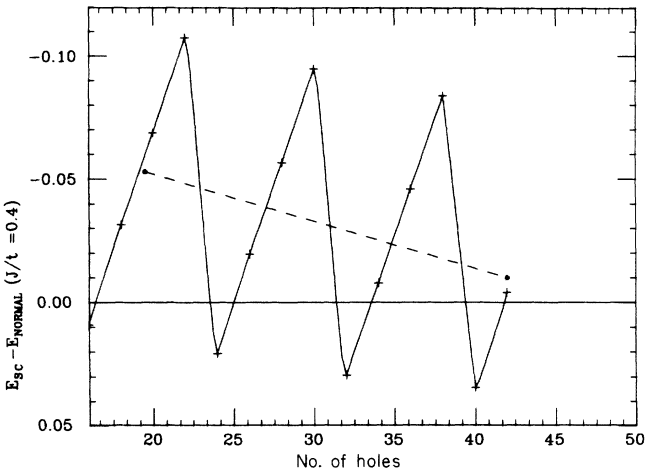

FIG. 4. Total-energy difference in units of t between superconducting and Fermi-liquid state for different doping levels. The curved line is a guide to the eye. The straight line represents an attempt to smooth the data in order to eliminate finite-size-shell effects. The simulations in this region were performed on a 122-site lattice with 8×10^5 Monte Carlo steps.

The theoretical boundary between normal and superconducting states is probably at somewhat higher δ than the experiments give, although this is hard to measure in both the calculations and in the experiments. We obtained this boundary by assuming the normal state to be a Fermi liquid. As noted above, this may be questionable in view of the rather anomalous properties of the normal state. If indeed the Fermi liquid is unstable with respect to some other exotic but normal liquid, then the energy balance between the latter and the superconducting phase would move the phase boundary to lower δ.

This research was supported by the NSF under Grants No. DMR-8913862 and No. DMR-8812852. We would like to thank T. M. Rice for helpful discussions.

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