PHYSICAL REVIEW B VOLUME 40, NUMBER 4 1 AUGUST 1989

Mean-field theory for the t-J model

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(Received 14 April 1989)

We present a new mean-field theory for the t-J model using a representation in which singly occupied sites or spins are represented by bosons and empty sites or holes by fermions. We obtain a phase diagram which includes ferromagnetic, antiferromagnetic, spiral (with the pitch inversely proportional to the density of holes), and disordered spin-liquid phases, with a clear separation of charge and spin excitations. We comment on the conditions for obtaining superconductivity in the model.

There is considerable recent interest[1-10] in the properties of the t-J model, which can be represented by the Hamiltonian[1]

$$H=-t\sum_{\langle ij\rangle}\mathbf{P}c_{i\mu}^{\dagger}c_{j\mu}P-\frac{J}{2}\sum_{\langle ij\rangle}\mathbf{P}(\mathbf{C}_{ij}^{\dagger}\mathbf{C}_{ij})\mathbf{P}\,. \tag{1}$$

Here $\mathbf{C}_{ij}^{\dagger}\equiv c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}-c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger}$ creates a *singlet* pair of spins on nearest neighbors $\langle ij\rangle$, and $\mathbf{P}$ is the projection operator that eliminates double occupancy of sites. The second term is simply the superexchange interaction $-\frac{1}{2}J(\vec{\mathbf{S}}_i\cdot\vec{\mathbf{S}}_j-\frac{1}{4}n_in_j)$, where $\vec{\mathbf{S}}_i(\equiv\frac{1}{2}c_{i\mu}^{\dagger}\vec{\sigma}_{\mu\nu}c_{i\nu})$ and $n_i(\equiv c_{i\mu}^{\dagger}c_{i\mu})$ are the spin and number operators at site i. The first term permits motion of holes (or spins). As is well known, the above model is the effective Hamiltonian for the large-U Hubbard model,[1,11] with $J=4t^2/U$. Recent interest in this model[1-10] was stimulated by Anderson's suggestion[1] that it contains the physics of the CuO_2 layers in the high-T_c materials.[12] Zhang and Rice[13] have argued that such a model can be derived from a multiband Hubbard model[14] for the CuO_2 layers. Thus one would like to understand the properties of this model, in particular its phases and whether it exhibits superconductivity, as a function of t/J, the temperature T, and the filling factor δ (defined as the deviation from half filling, or the fractional number of empty sites).

The central result of this paper is that an elegantly simple mean-field theory takes into account the crucial competing spin correlations in the model and the way they affect and in turn are affected by the motion of holes. Specifically, we obtain a $T=0$ phase diagram with four phases, a "ferro" metallic phase with long-range ferromagnetic order for $t\delta\gg J$, an "antiferro" insulating phase for $t\ll J$ and δ not too large, a "disordered spin-liquid" insulating phase with only short-range antiferromagnetic correlations for $t\ll J$ and δ large, and a "spiral" metallic phase with long-range spiral (incommensurate) spin order[7] when $t\delta\sim J$. The results are summarized in Fig. 1, and discussed in more detail below. While these phases have been obtained in several papers,[15] using various separate approximate methods, ours is the first simple mean-field theory that obtains all of them in a single scheme and permits detailed calculations in the incommensurate phase. We also discuss preliminary results for the conditions for obtaining superconductivity in this model.

Our new mean-field theory for the t-J Hamiltonian uses the representation: $c_{i\mu}^{\dagger}=b_{i\mu}^{\dagger}f_i$ where $b_{i\mu}^{\dagger}$ are Schwinger-boson operators which represent the spins[16] $\vec{\mathbf{S}}_i(=\frac{1}{2}b_{i\mu}^{\dagger}\vec{\sigma}b_{i\nu})$ and f_i are hole-fermion operators which represent the empty sites. There is a local constraint $b_{i\mu}^{\dagger}b_{i\mu}+f_i^{\dagger}f_i=1$ which has to be imposed to preserve the Hilbert space, but we impose this only on an average as in all such mean-field theories.[2-6] In this representation (1) can be written[17]

$$H=-2t\sum_{\langle ij\rangle}(\mathbf{B}_{ij}^{\dagger}f_j^{\dagger}f_i+\text{H.c.})-2J\sum_{\langle ij\rangle}(1-f_i^{\dagger}f_i)\mathbf{A}_{ij}^{\dagger}\mathbf{A}_{ij}(1-f_j^{\dagger}f_j)\,, \tag{2}$$

$$\mathbf{B}_{ij}^{\dagger}\equiv\frac{1}{2}\sum_{\sigma}b_{i\sigma}^{\dagger}b_{j\sigma},\quad \mathbf{A}_{ij}^{\dagger}\equiv\frac{1}{2}\sum_{\sigma}\sigma b_{i\sigma}^{\dagger}b_{j-\sigma}^{\dagger}\,. \tag{3}$$

Our choice of representation and the mean-field theory has the following features. Exactly at half filling ($\delta=0$) our theory reduces to the Schwinger-boson large-N theory recently studied by Arovas and Auerbach[18] and later extended by us.[19] Arovas and Auerbach showed that a mean-field theory with $\langle\mathbf{A}_{ij}\rangle\neq0$ for the quantum antiferromagnet, and with $\langle\mathbf{B}_{ij}\rangle\neq0$ for the quantum ferromagnet, gives a surprisingly good account of the "spin-liquid" (i.e., strongly correlated but disordered) phase, especially in low dimensions. In our extension, we have shown that this theory can account for long-range magnetic order in these models, provided we associate the magnetic ordering with a Bose condensation of the Schwinger bosons. This theory correctly reproduces the spin-wave theory results for the low-temperature magnetization and the spin-wave

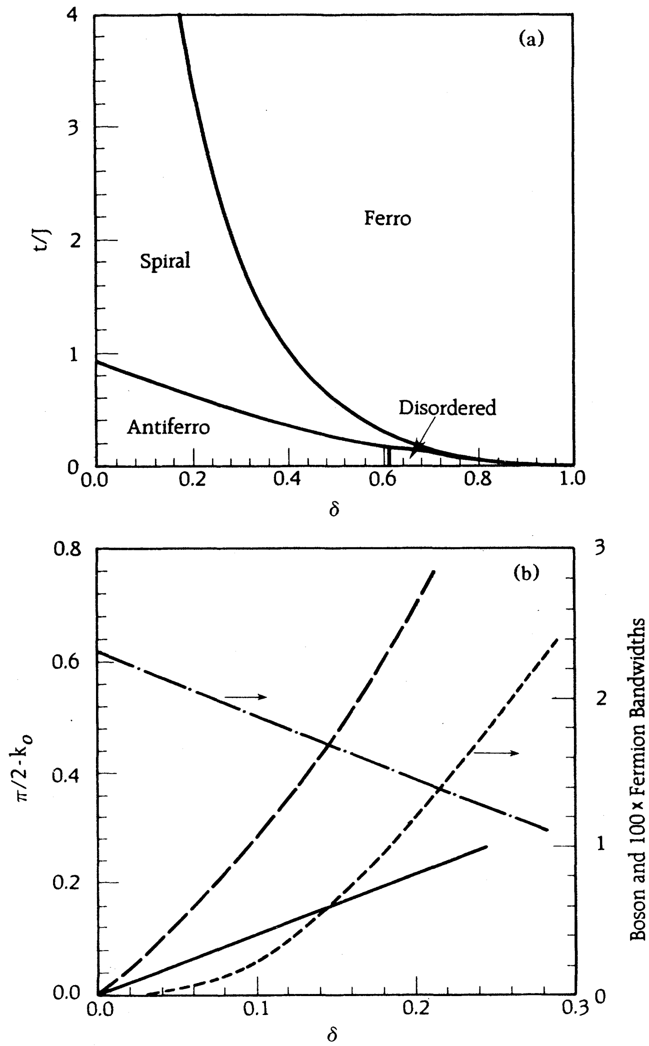

FIG. 1. (a) Phase diagram of the t-J model on a square lattice at $T=0$ in our mean-field theory showing the antiferro, ferro, disordered spin liquid, and spiral phases. See text for discussion. (b) Variation of $(\pi/2)-k_0$ as a function of δ along the antiferro-spiral phase boundary (solid line) and at $t/J=1.96$ (long-dashed line). Also shown are the boson bandwidth (dash-dotted line) and $100\times$fermion bandwidth (short-dashed line) along the antiferro-spiral phase boundary, in units of J.

spectrum. This is different from the results obtained in the fermionic representation, and hence we favor the bosonic representation of spins over the fermion. Furthermore, the mean-field decomposition of the hole hopping term t ties together hole mobility and short-range ferromagnetic correlations, which is the physics discussed by Nagaoka[20] for the $U=\infty$ Hubbard model.

Specifically, we do a simple Hartree-Fock factorization of (2) using $\langle \mathbf{A}_{ij}\rangle$, $\langle \mathbf{B}_{ij}\rangle$, and $\langle f_i^\dagger f_j\rangle$ as the mean-field amplitudes. [This is equivalent to doing a Peierls variational calculation or to the $n\rightarrow\infty$ limit of an appropriate large n generalization of (2).] We take into account the (average) constraint $\langle(\sum_\sigma b_{i\sigma}^\dagger b_{i\sigma}+f_i^\dagger f_i)\rangle=1$ and the filling factor $\langle f_i^\dagger f_i\rangle=\delta$ via (Lagrange multiplier) chemical potentials λ and μ, respectively. We find that the following simple choice for the mean-field amplitudes,

$$\langle \mathbf{A}_{ij}\rangle = iA\sin(\vec{Q}\cdot\vec{r}_{ij}/2),\quad \langle \mathbf{B}_{ij}\rangle = B,\quad \langle f_i^\dagger f_j\rangle = D\,, \tag{4}$$

where $\vec{Q}$ denotes the zone-corner wave vector, captures the essential physics of competing spin correlations and hole motion. In particular, as we show below, a nonzero value for A corresponds to short-range antiferromagnetic correlations, and for B to ferromagnetic correlations; a nonzero value of D implies hole mobility.

The resulting mean-field Hamiltonian is quadratic in the Bose and Fermi operators and can be easily diagonalized (the Bose part by a Bogoliubov transformation). We find propagating fermionic and bosonic quasiparticles with dispersions

$$\epsilon_k = (2tB+2JRD)z\gamma_k - \mu\,, \tag{5}$$

$$\omega_k = [(\lambda+d\gamma_k)^2-(a\phi_k)^2]^{1/2}\,, \tag{6}$$

respectively. Here z is the coordination number, $d\equiv(tD+JPB/2)z$, $a\equiv JAPz$, $\gamma_k\equiv(2/z)\sum_{\vec\delta}\cos\vec{k}\cdot\vec{\delta}$, and $\phi_k\equiv(2/z)\sum_{\vec\delta}\sin\vec{k}\cdot\vec{\delta}$. R and P are expectation values given by $R\equiv\langle \mathbf{A}_{ij}^\dagger \mathbf{A}_{ij}\rangle$ and $P\equiv\langle(1-f_i^\dagger f_i)(1-f_j^\dagger f_j)\rangle$. Using these we derive self-consistent equations for A, B, D, λ, and μ, and solve them numerically for the lowest free-energy solution for various values of t/J, δ, and T. In this paper for the most part we discuss $T=0$ results for the square lattice.

One important component of the physics contained in our mean-field theory is brought out by the spin-spin correlation function, which is given by (for $r_i\neq r_j$)

$$\langle S_i^+S_j^-\rangle = f(r_{ij})f^*(r_{ij})+g(r_{ij})g^*(r_{ji})\,, \tag{7}$$

$$\begin{pmatrix} f(r_{ij}) \\ g(r_{ij})\end{pmatrix} = \sum_k e^{-i\vec{k}\cdot\vec{r}_{ij}}\begin{pmatrix}\cosh 2\theta_k \\ \sinh 2\theta_k\end{pmatrix}[n(\omega_k)+\tfrac{1}{2}]\,, \tag{8}$$

where $n(\omega_k)=(e^{\beta\omega_k}-1)^{-1}$ is the Bose-distribution function and $\tanh 2\theta_k=-a\phi_k/(\lambda+d\gamma_k)$ is the Bogoliubov parameter. When i and j are nearest neighbors it is easy to show that $f(r_{ij})=f^*(r_{ji})=B$ and $g(r_{ij})=-g^*(r_{ji})=A$, and thus $\langle S_i^+S_j^-\rangle\sim(B^2-A^2)$. Hence the result that A promotes short-range antiferromagnetic correlations and B short-range ferromagnetic correlations. From our self-consistent mean-field equations we find that a nonzero value of B implies a nonzero value of D and vice versa. Thus the correlation of hole motion with ferromagnetic correlations discovered by Nagaoka is automatically included in our simple mean-field theory.

The short-range correlations determined by A and B set in at high temperatures, governed by t and J. At these temperatures our self-consistent equations show that λ is such that ω_k has a gap. Hence from (7) and (8) it follows that the spin correlations decay exponentially at long distances and the system has no long-range spin order.

However, at low temperatures (T less than a critical temperature T_c in three dimensions, and at $T=0$ in two dimensions), the physics is dominated by Bose condensation of the Schwinger bosons, which leads to long-range spin order. This arises because the chemical potential λ, and hence, the minimum of ω_k given by (6) decrease as the temperature decreases. When $\lambda=\lambda_c=(d^2+a^2)^{1/2}$, ω_k develops zero modes at wave vectors $\pm\vec{k}_0=\pm k_0(1,1,\ldots)$ with $\cos k_0=-d/\lambda_c$ and $\sin k_0=a/\lambda_c$. The Bose condensation of these modes leads to off-diagonal-long-range order in the spin-spin correlations function in (7) given by

$$\langle S_i^+ S_j^-\rangle_{r_{ij}\to\infty}=\rho_0^2\cos(2\vec{k}_0\cdot\vec{r}_{ij})\,. \tag{9}$$

For a general $k_0(\neq\pi/2$ or $0)$ this represents a spiral spin order with wave vector $2\vec{k}_0$ and magnetization ρ_0, which goes continuously into ferromagnetic order in the limit $k_0\to 0$, and to Néel antiferromagnetic order in the limit $k_0\to\pi/2$.

Figure 1(a) shows our results for the phase diagram[21] for the t-J model on a square lattice at zero temperature. In the region marked ferro, the minimum energy solution has $A=0$ and $B,D\neq 0$ implying $k_0=0$ and ferromagnetic long-range order. The effective ferromagnetic coupling is $J_F=-tD\sim t\delta(1-\delta)$, and the condensate density is $\rho_0^F=(1-\delta)/2$, which corresponds to the maximum alignment of the $1-\delta$ occupied sites. The holes move freely with an effective bandwidth of $tB=t(1-\delta)/2$. In the region marked antiferro, the minimum energy solution has $B=D=0$, and $A\neq 0$. This yields $k_0=\pi/2$ and corresponds to a Néel state. Here (at the mean-field level) the holes are localized,[22] since t is not large enough to make the energy gain due to hole motion win over its frustrating effect on the antiferromagnetic order and the consequent loss of exchange energy. The effective antiferromagnetic coupling is $J_A=J(1-\delta)^2$, and the $T=0$ staggered magnetization is $\rho_0^A=(1-\delta/2)-\frac{1}{2}\int_k(1-\gamma_k^2)^{-1/2}$. In the region marked spiral, A, B, and D are nonzero, and $0<k_0<\pi/2$, and the ground state has spiral spin order. The spiral magnetization is given by

$$\rho_0^S=(1-\delta/2)-\frac{1}{2}\int_k(1+\alpha\gamma_k)[(1+\alpha\gamma_k)^2-\eta^2\phi_k^2]^{-1/2}\,,$$

where $\alpha=-\cos k_0$ and $\eta=\sin k_0$. As $\delta\to 0$, $k_0\to\pi/2$ and the spiral phase goes continuously into the antiferromagnetic phase at half filling. When δ becomes very large for small t/J, the system is unable to sustain the Bose condensation. Hence the long-range order disappears, and one is left with a disordered spin-liquid phase with just short-range (antiferromagnetic) correlations.

For small δ the deviation of k_0 from $\pi/2$, i.e., the inverse of the pitch of the spiral scales with δ as shown in Fig. 1(b). The figure also shows the boson and fermion bandwidths as a function of δ. Note that for small δ the charge excitations are heavy (small-fermion bandwidth) and the spin excitations are light.[23]

Consider the question of superconductivity in the t-J model. For spin-singlet superconductivity one needs $\langle\sum_\sigma c_{i\sigma}^\dagger c_{j-\sigma}^\dagger\sigma\rangle\equiv\langle A_{ij}^\dagger f_i f_j\rangle$ to be nonzero. Within our mean-field picture, this requires *both* $\mathbf{A}_{ij}\neq 0$, i.e., short-range antiferromagnetic correlations *and* $\langle f_i f_j\rangle\neq 0$, i.e., two-hole fermions must bind. The hole binding can come about by attractive interactions generated by (spin) fluctuations of the Schwinger bosons. A preliminary analysis of these interactions due to Gaussian fluctuations about our mean-field theory indicates that optimal conditions for superconductivity occur when $t\approx J$ and δ intermediate.

Our mean-field theory overestimates the stability of the ferromagnetic phase. It has recently been demonstrated[24] that the Nagaoka state is unstable for large δ and finite U (which corresponds to finite J) due to "Fermi-surface restoring" spin-wave excitations with wave vector k_F. We anticipate that incorporation of such excitations into our mean-field theory will get rid of the ferromagnetic long-range order in the bulk of the region marked ferro, and replace it by a disordered spin-liquid phase. Also, fluctuations about our mean-field solution promote hole mobility even in the antiferro phase, and hence may favor the spiral phase at its expense. Fluctuation effects are also responsible for superconducting paring between the holes. We believe that the incorporation of these effects with the above mean-field theory as the starting point will yield a viable theory of the t-J model for all ranges of its parameters.

We have also studied the finite-U Hubbard model using methods similar to those described above, where we introduce an additional fermion operator d_i to represent doubly occupied sites. The resulting mean-field theory yields the same results as described above in the large-U limit, and also leads to a theory for the metal-insulator transition in the half-filled case.

C.J. and H.R.K. acknowledge financial support from the National Science Foundation (Grant No. NSF-DMR 8451911). The research of H.R.K. and S.S. was supported in part by a grant from the U.S. Department of Energy–Basic Energy Sciences, Division of Materials Research. H.R.K. thanks P. W. Anderson for several stimulating discussions and support through Grant No. NSF-DMR 8518163.

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[17]Note that the factors of $(1-f_i^{\dagger}f_i)$ in Eq. (2) can be replaced by 1 if the constraint is imposed exactly at every site. However, since in our theory we treat the constraint only on an average, we have found it useful to keep these factors and treat them in a mean-field approximation as well. We thus take into account in an average, statistical way the reduction in the number of "J bonds" (where J acts) when holes are present.

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[21]We have checked the stability of our phase diagram with respect to some other simple choices of the mean-field amplitudes which allow for the possibility of long-range ferrimagnetic order in addition to the ferro- and antiferromagnetic phases. We find that the spiral phase is lower in energy than the ferrimagnetic phase.

[22]If one includes a pair-hopping term (see Ref. 11) characteristic of the large-U Hubbard model *and* allows t/J to be arbitrary then the holes will be mobile with a bandwidth proportional to $J(1-\delta)^2$ in the antiferromagnetic and disordered phases and these phases are metallic even in the mean-field theory.

[23]P. W. Anderson (private communication) has suggested that the normal phase of the cuprate superconductors has a large specific heat and a small susceptibility, and that heavy charge excitations and light spin excitations are responsible for such a result.

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