Small-Polaron Theory of Doped Antiferromagnets

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The spin-hole coherent-state path integral is used to generate a systematic large-spin expansion of the t-J model on the square lattice. The single hole's classical energy is minimized by small polarons with short-ranged interactions. Intersublattice hopping of polarons is forbidden by a tunneling selection rule. We derive the low-energy Lagrangian which reduces to the model of Wiegmann, Wen, Shankar, and Lee of Néel-gauge-field-induced superconductivity.

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The discovery of high-temperature superconductivity has spurred intense investigations of the two-dimensional doped antiferromagnet. In the strong-coupling limit, the t-J Hamiltonian, derived from the large-U Hubbard model,[1] is often used to describe the low-lying excitations. At zero doping, it directly reduces to the quantum antiferromagnetic Heisenberg model (QHM). Substantial progress has been recently achieved in understanding the Heisenberg limit, both theoretically and experimentally.[2] The effects of doping, however, are still highly controversial.

Continuum theories[3] and the Schwinger-boson–slave-fermion mean-field theory[4] predict spiral magnetic phases at finite doping concentrations. Recently, however, the RPA determinant has been found to be unstable (negative) in a *range of momenta.*[5] The offending fluctuations were identified as local enhancements of the spiral distortion. Clearly, the holes drive strong perturbations of the spins on the lattice-constant scale. These are difficult to treat by direct application of continuum and mean-field approximations on the Hubbard and t-J models.

The path integral of spin coherent states has been fruitfully used by Haldane to map the QHM onto the nonlinear σ model and to derive the topological Berry phases.[6] It provided a unified semiclassical treatment of the ordered and disordered phases of the quantum antiferromagnet. In this Letter we generalize this path integral to represent the t-J model by defining "spin-hole coherent states." This allows us to treat the short-range interactions carefully, while observing the local constraints. We derive a semiclassical expansion of the ground state and low excitations in the presence of holes. Although the expansion is formally controlled by the large spin size S we have learned that (at least for the undoped case[2]) it can work well even for $S=\frac{1}{2}$.

The t-J Hamiltonian is given by[5]

$$\mathcal{H}^{tJ}=t\sum_{\langle i;j\rangle}f_i^\dagger f_j\mathcal{F}_{ij}-\frac{J}{4}\sum_{\langle i;jk\rangle}(\delta_{ik}-f_k^\dagger f_i)\mathcal{A}_{ij}^\dagger\mathcal{A}_{kj}(1-f_j^\dagger f_j)\,, \tag{1}$$

where $\mathcal{A}_{ij}^\dagger\equiv(a_i^\dagger b_j^\dagger-b_i^\dagger a_j^\dagger)$ and $\mathcal{F}_{ij}^\dagger\equiv(a_j^\dagger a_i+b_j^\dagger b_i)$. $\langle i;j\rangle$ ($\langle i;jk\rangle$) denote summation over sites i and their first (second) nearest neighbors on the square lattice. $J=4t^2/U$ is the Heisenberg superexchange constant. t and U are the hopping and interaction parameters of the parent Hubbard model. Equation (1) includes *all the terms* to second order in t/U. The operators a_i,b_i (f_i) are Schwinger bosons (slave fermions), and the Hilbert space is subjected to the constraint $a^\dagger a+b^\dagger b+f^\dagger f=2S$ at each site. This constraint generalizes the original Hubbard $S=\frac{1}{2}$ states to arbitrary spin S.

The spin-hole coherent states are defined as follows:

$$|\hat{\mathbf{\Omega}},\xi\rangle_S=|\hat{\mathbf{\Omega}}_S\rangle|0\rangle+|\hat{\mathbf{\Omega}}_{S-1/2}\rangle\xi f^\dagger|0\rangle\,. \tag{2}$$

$|\hat{\mathbf{\Omega}}_S(\theta,\phi)\rangle=(2S!)^{-1/2}(ua^\dagger+vb^\dagger)^{2S}|0,0\rangle$ are the standard spin coherent states, where $u=\cos(\theta/2)e^{-i\phi/2}$ and $v=\sin(\theta/2)e^{i\phi/2}$. ξ is a Grassman variable. The states (2) allow a resolution of the identity in the S sector:

$$\frac{2S}{4\pi}\int d\phi\, d\cos\theta\, d\xi^*\, d\xi\exp(-\alpha_S\xi^*\xi)|\hat{\mathbf{\Omega}},\xi\rangle\langle\hat{\mathbf{\Omega}},\xi|=I\,, \tag{3}$$

where the factor $\alpha_S=(2S+1)/2S$ is required for normalizing the matrix elements to unity. In the grand canonical partition function, α_S is replaced by unity by renormalizing the chemical potential μ.

Following standard procedure[6] we use (3) to construct the path integral for the partition function:

$$Z=\int\mathcal{D}\hat{\mathbf{\Omega}}\,\mathcal{D}\xi^*\,\mathcal{D}\xi\exp\left[\int_0^\beta d\tau\sum_i[i(2S-\xi_i^*\xi_i)\mathbf{A}(\hat{\mathbf{\Omega}}_i)\cdot\dot{\hat{\mathbf{\Omega}}}_i+\xi_i^*\dot{\xi}_i]-H^{tJ}[\hat{\mathbf{\Omega}},\xi^*,\xi]\right]. \tag{4}$$

H^{tJ} in (4) is given by Eq. (1) where $a,b,f\to u,v,\xi$. $\mathbf{A}\cdot\dot{\hat{\mathbf{\Omega}}}_i$ is the spin-kinetic term, where $\mathbf{A}(\Omega)$ is the vector potential of a unit magnetic monopole at the origin $\Omega=0$. The fermion "time derivatives" denote the discrete form

$\dot{\xi}=[\xi(\tau)-\xi(\tau-\epsilon)]/\epsilon$, where ϵ is the time step.

H^{tJ} has quadratic and quartic fermion terms. We decouple the four-fermion terms by the Hartree-Fock approximation. For our purposes this approximation is justified by the following arguments: (i) Hole-correlation corrections are of higher order in hole density, and (ii) the quartic terms vanish in the ferromagnetically correlated regions, where the hole density is high. We define $\rho_{ij}[\hat{\mathbf{\Omega}}]=\langle f_i^\dagger f_j\rangle$ to be determined self-consistently, and write $H^{tJ}\approx\overline{H}^J+\overline{H}^f-\mu\sum_i\xi_i^*\xi_i$ where

$$\overline{H}^J=-\frac{\bar{J}}{8}\sum_{\langle i;jk\rangle}(\delta_{ik}-e^{i\psi_{ik}}\rho_{ik}\rho_{jj})[(1-\hat{\mathbf{\Omega}}_j\cdot\hat{\mathbf{\Omega}}_k)(1-\hat{\mathbf{\Omega}}_i\cdot\hat{\mathbf{\Omega}}_j)]^{1/2},$$
$$\overline{H}^f=\frac{\bar{t}}{\sqrt{2}}\sum_{\langle i;j\rangle}(1+\hat{\mathbf{\Omega}}_i\cdot\hat{\mathbf{\Omega}}_j)^{1/2}e^{i\gamma_{ij}}\xi_i^*\xi_j+\frac{\bar{J}}{8}\sum_{\langle i;jk\rangle}[(1-\hat{\mathbf{\Omega}}_j\cdot\hat{\mathbf{\Omega}}_k)(1-\hat{\mathbf{\Omega}}_i\cdot\hat{\mathbf{\Omega}}_j)]^{1/2}[(1-\rho_{jj})e^{i\psi_{ik}}\xi_i^*\xi_k+(\delta_{ik}-e^{i\psi_{ik}}\rho_{ik})\xi_j^*\xi_j]. \tag{5}$$

Here we define the *classical* parameters $\bar{J}\equiv 4JS^2$ and $\bar{t}\equiv 2tS$. The sums in $\overline{H}^f$ represent two distinct hopping processes: intersublattice hopping ("t terms") and intrasublattice hopping ("J terms"). γ_{ij} and ψ_{ik} are the phases of $u_i^*u_j+v_i^*v_j$ and $(u_i^*v_j^*-v_i^*u_j^*)(u_kv_j-v_ku_j)$, respectively. When the spins $\hat{\mathbf{\Omega}}_i$ have short-range antiferromagnetic order the γ phases in the t terms fluctuate wildly, while $\psi_{ik}=\eta_i\mathbf{A}^N\cdot(\mathbf{x}_i-\mathbf{x}_k)$ represents a slowly varying Néel gauge field $\mathbf{A}^N(\mathbf{x})$ whose curl is the topological density of the staggered magnetization.[7] $\eta_i=+1$ (-1) on sublattice A (B) is the corresponding "sublattice charge." Weigmann, Wen, Shankar, and Lee have studied Lagrangians which contain similar intrasublattice $\mathbf{A}^N$-coupled hopping terms in the context of high-T_c superconductivity.[8] Returning to the t-J model, we see that the t terms are not $\mathbf{A}^N$-gauge invariant, *and do not conserve the sublattice charges.* Although the t terms cannot be justifiably ignored, especially in the $\bar{t}/\bar{J}>1$ regime, we shall soon see how they are effectively eliminated from the low-energy Lagrangian.

We begin by integrating out the fermions to obtain a spin partition function

$$Z^s=\int\mathcal{D}\hat{\mathbf{\Omega}}\exp\left[\int_0^\beta d\tau\left(i\sum_i(2S-\rho_i)\mathbf{A}(\hat{\mathbf{\Omega}}_i)\cdot\dot{\hat{\mathbf{\Omega}}}_i-\overline{H}^J[\hat{\mathbf{\Omega}}]-E^f[\hat{\mathbf{\Omega}}]\right)\right], \tag{6}$$

where $E^f[\hat{\mathbf{\Omega}}]$ is the time-retarded action (free energy) of the Hamiltonian $\overline{H}^f$. Here we concentrate on the zero-temperature case $\beta=\infty$. Equation (6) is a useful starting point for the semiclassical approximation. In the classical limit, $S\to\infty$, the spins are frozen, i.e., $\langle\dot{\hat{\mathbf{\Omega}}}\rangle=0$. The first step is to minimize $\overline{H}^J+E^f$ for a given number of holes. The second step includes the semiclassical fluctuations whose dynamics are given by the kinetic terms. We discuss the single-hole and the many-hole cases separately.

The single hole.—In the regime $\bar{t}/\bar{J}>0.87$, the "polaron," which is a *local* alignment of spins, yields a lower energy than any of the possible uniform states, including the Néel state, spiral states, and canted states. This result helps to explain the instability in the RPA fluctuations about the uniform states.[5]

We used a Lanzcos algorithm on the Connection Machine to minimize the energy for 128×128 spins. The polaron variational parameters were chosen to describe a ferromagnetic core, a transition region, and a far-field antiferromagnetic tail. The latter is completely determined by the boundary condition $\delta\theta$ and the pure Heisenberg model (i.e., the Laplace equation).

Our results are quite simple. For $1<\bar{t}/\bar{J}<4.1$ the single-hole energy is minimized by the five-site polaron (one flipped spin), depicted in Fig. 1. The hole density is approximately $\frac{1}{2}$ and $\frac{1}{8}$ on the central and neighboring sites, respectively, with a small amount of leakage [due to the J terms in (5)] to sites further away. For $4.1<\bar{t}/\bar{J}<6.6$, the polaron has two flipped spins (diagonally across a plaquette), and at larger values the core radius increases slowly as $R_c\sim(\bar{t}/\bar{J})^{1/4}$, and the energy goes asymptotically as $\epsilon_h+4\bar{t}\sim(\bar{J}\bar{t})^{1/2}$. The most important fact is that the small polarons *do not distort the Néel background.* In particular, the configurations centered on a bond[9] are considerably higher in energy. We also find that the polarons have no tails,[3] i.e., $\delta\theta=0$, throughout the regime discussed above. This follows from competing contributions of order $\pm\bar{J}(\delta\theta)^2$ of $\overline{H}^J$ and E^f. Since, in addition, the density ρ is exponentially localized near the polaron sites, we conclude that *the classical interactions between polarons are short ranged.*

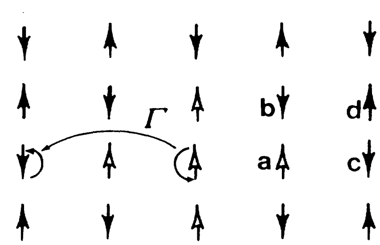

FIG. 1. The five-site polaron. The hole density is primarily concentrated on the sites of the unfilled arrows. The circular arrows represent an allowed tunneling path, where the polaron hops two lattice constants to the left. Γ is the hopping rate given by Eq. (7).

The polaron breaks the lattice translational symmetry. This symmetry is restored by tunneling events, where two spins i and k simultaneously flip their orientation (see Fig. 1). The tunneling matrix element Γ_{ik} (the polaron's hopping rate) is nonperturbative in S^{-1}:

$$\Gamma_{ik} = \Gamma_0 \exp\left(-\sum_{i'} \int d\tilde{\phi}_{i'} \bar{S}^z_{i'}\right) \approx S^{1/2} \beta_{ik} \bar{t} \exp(-S\alpha_{ik}) . \tag{7}$$

Equation (7) can be computed as follows: The azimuthal coordinates are analytically continued $i\phi \to \tilde{\phi}_i$, while their cannonical momenta $S^z_i = (2S - \rho_i)\cos\theta_i$ are kept real. It can be readily verified that $\sum_i S^z_i$ and $\bar{H}^J + E^f$ are conserved along the tunneling path $\bar{S}^z_i(\tilde{\phi})$ which minimizes the action. As a result of these conservation laws, we obtain a selection rule: *Tunneling can only take place between sites on the same sublattice.* This, in effect, amounts to the elimination of the intersublattice t terms.

α_{ik}, β_{ik} are slowly varying dimensionless functions of $\bar{t}$ and $\bar{J}$. For five-site polarons and $S = \frac{1}{2}$ we estimate the exponent to be roughly unity, but a fuller treatment of the multidimensional tunneling problem is required for a quantitative determination of the polaron's effective mass.

The single polaron in a perfect Néel background occupies a Bloch wave of dispersion

$$\epsilon_{\mathbf{k}} = 2\Gamma_c[\cos(2k_x) + \cos(2k_y)] + 2\Gamma_b[\cos(k_z + k_y) + \cos(k_x - k_y)] ,$$

where c,b denote the site of the other flipped spin as labeled in Fig. 1. By energetic arguments, $\Gamma_b \le \Gamma_c$. Thus the single-polaron energy is minimized at $\mathbf{k} = (\pi/2, \pi/2)$. This result agrees with other studies of the single-hole spectral function in the t-J model.[10] For small deviations of the background spins from antiferromagnetic order the tunneling rate Γ_{ik} is modulated by the overlap of the background and the perfectly antiferromagnetic configurations. This overlap is just $\exp[i\eta_i \mathbf{A}^N \cdot (\mathbf{x}_i - \mathbf{x}_k)]$. $\mathbf{A}^N$ and η_i are the aforementioned Néel gauge field and sublattice charge, respectively. *We notice that* $\mathbf{A}^N$ *couples in a gauge-invariant way to the polarons, and that the sublattice charges are conserved in the hopping.*

Interactions.—The interactions between two polarons were computed in the regime $\bar{t}/\bar{J} = 1$-4. We define $U^p_{ij} = \frac{1}{2} e_{ij} - 2e_h$, where e_{ij} is the relaxed energy of a two-hole polaron with flipped spins at sites i and j. U^p_{ii} is repulsive, and of order $0.6\bar{J}$-$2.6\bar{J}$. The intersite interactions, for neighboring polarons at sites a-d (see Fig. 1), are plotted in Fig. 2. We find both attractive and repulsive interactions, and it is interesting to note that for $\bar{t}/\bar{J} < 1.8$ there is a near-neighbor attraction of antiferromagnetically correlated spins. We also consider the possibility of polaron condensation into hole-rich domains.[11] The condensation energy per hole is determined by minimizing it with respect to the spin configuration, and the density. The spins in the hole-rich domains align ferromagnetically, and the energy per hole is given by $e_{\mathrm{fm}} = -4\bar{t} + 4(B\bar{J}\bar{t}\pi)^{1/2}$. This result coincides with that of Emery, Kivelson, and Lin,[11] except that their quantum correction factor $B = 0.584$ is here set to $\frac{1}{2}$. In Fig. 2, the condensation energy $\Delta e_c = e_{\mathrm{fm}} - e_h$ is plotted. We find that it becomes negative at $\bar{t}/\bar{J} = 2.7$, *above which phase separation will occur for large S.*

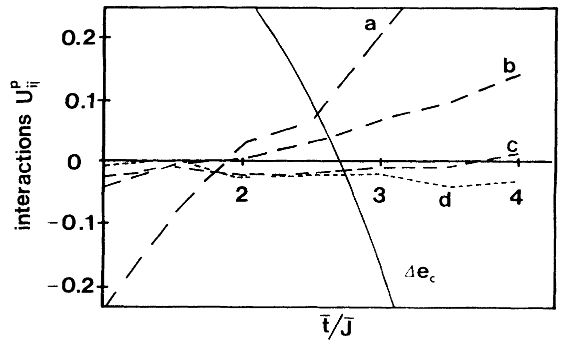

FIG. 2. Classical interactions between polarons, in units of $\bar{J}$. Lines a-d represent the second polaron positions as labeled in Fig. 1. The solid line represents the relative condensation energy per hole of the hole-rich phase (see text).

Attractive interactions and negative condensation energies may result in charge-density waves or superconductivity in the ground state of the quantized model. However, if realistic intersite Coulomb repulsions are added to the t-J model, the attractive interactions may change sign. In particular, phase separation will be suppressed, or pushed to higher values of $\bar{t}/\bar{J}$.

The information given above allows us to write the effective Lagrangian for a dilute system of small polarons:

$$\mathcal{L}^{s\text{-}p} = \sum_i [i(2S - p_i^* p_i)\mathbf{A}(\hat{\mathbf{\Omega}}_i) \cdot \dot{\hat{\mathbf{\Omega}}}_i + p_i^* \dot{p}_i] + \frac{\bar{J}}{8} \sum_{\langle i;j \rangle} \hat{\mathbf{\Omega}}_i \cdot \hat{\mathbf{\Omega}}_j + \sum_i (e_h - \mu) p_i^* p_i + \sum_{\langle i;jk \rangle} \Gamma_{ik} e^{\eta_i \mathbf{A}^N \cdot \mathbf{x}_{ik}} p_i^\dagger p_k + \sum_{ij} U^p_{ij} p_i^* p_i p_j^* p_j . \tag{8}$$

Equation (8) is the main result of this paper. $\mathcal{L}^{s\text{-}p}$ describes a two-charge system of spinless fermions p_i with short-range interactions U^p_{ij} coupled to Heisenberg spins. The formation of polarons can be viewed as a strong short-wavelength dressing of the original f holes by the spins. As a consequence, the uncomfortable t terms have been conveniently eliminated, and the effect of holes on the spin background is short ranged. A major advantage of the model (8) over Eq. (5) is that in the small concentration limit $\delta \ll 1$, (8) is amenable to the continuum approximation. Following Haldane[6] the spin interactions can be relaced by the $(2+1)$-dimensional nonlinear σ model, with δ-dependent renormalized stiffness constant and spin-wave velocity. The precise evaluation of the σ-model parameters for finite δ is beyond the scope of this paper, but we expect that above some critical density $\delta > \delta_c$ the ground state is disordered;[12] i.e., a "spin liquid." In the massive spin-liquid phase, Eq. (8) reduces to Wiegmann, Wen, Shankar, and Lee's model:[8]

$$\mathcal{L}^{\mathrm{WWSL}} = \sum_{\eta=\pm 1} \left[p_\eta^\dagger (\partial_\tau + i\eta A_0^N) p_\eta + \frac{1}{2m} p_\eta^\dagger |\nabla + i\eta \mathbf{A}^N|^2 p_\eta \right] + \frac{1}{4\kappa}(F_{\mu\nu})^2 + \mathcal{O}(p^\dagger p p^\dagger p) \cdots , \tag{9}$$

where m is the effective mass at $\mathbf{k}=(\pi/2,\pi/2)$, and the "electromagnetic" Néel fields are $F_{\mu\nu} = \partial_\mu A_\nu^N - \partial_\nu A_\mu^N$. κ is the inverse spin correlation length, which is also the coupling constant of the gauge field. Previous analyses[8] have concluded that the ground state of (9) is most likely a resonating-valence-bond-type superconductor. Lee argued[8] that the pairing is caused by two effects: (i) attraction between the opposite charges induced by the Néel gauge field, and (ii) suppression of coherent single-particle propagation due to fluctuating Bohm-Aharonov phases, while the pairs $\langle p_+^\dagger p_-^\dagger \rangle$ propagate as free bosons. Both (i) and (ii) are only valid in the magnetically disordered phase, a pleasing feature which agrees with the phase diagrams of the copper-oxide superconductors.

Aside from the mechanism of superconductivity, the small-polaron theory could be checked numerically by finite-lattice Monte Carlo simulations, and experimentally in the copper oxides and other doped antiferromagnets. For example, the polaron size can be estimated by NMR techniques,[13] and its internal excitations could be probed by optical absorption. In the frozen-moments regime, one expects the polarons to exhibit conductivity typical of weakly localized semiconductors.[14]

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Note added.—In a recent paper,[15] Dagotto and Schrieffer have found that a quasiparticle state which describes a five-site polaron of momentum $\mathbf{k}=(\pi/2,\pi/2)$ has appreciable overlap with the exact ground state of the single-hole t-J model on a 4×4 lattice. The agreement with our semiclassical predictions validates the use of the large-S approximation to this model.

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