Metallic and magnetic properties of the t-J model: One-site approximation

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The t-J model is analyzed by means of the Caron-Pratt approximation. With the use of a self-consistent cluster calculation, the magnetic phase diagram and the temperature and hole-concentration dependence of the antiferromagnetic and metallic order parameters are obtained.

I. INTRODUCTION

The theory of strongly correlated fermion systems on a two-dimensional lattice has been developed currently in connection with high-T_c superconductivity.[1,2] The magnetic properties of the layered oxide superconductors with the CuO_2 plane should contain important information about the mechanism of high-temperature superconductivity. One of the simplified models which are considered to include the essential physics of these materials is the t-J model.[2] This model can be obtained as the large-U limit of the Hubbard model.[3-6] The t-J Hamiltonian is given by

$$H=-t\sum_{\langle ij\rangle\sigma} d_{i\sigma}^{\dagger}d_{j\sigma}+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)-\mu\sum_i n_i\ , \tag{1}$$

where $d_{i\sigma}^{\dagger}=(1-n_{i,-\sigma})c_{i\sigma}^{\dagger}$, $\mathbf{S}_i=\frac{1}{2}c_{i\alpha}^{\dagger}\boldsymbol{\sigma}^{\alpha\beta}c_{i\beta}$, and $n_i=\sum_\sigma c_{i\sigma}^{\dagger}c_{i\sigma}$. $c_{i\sigma}^{\dagger}$ creates an electron of spin σ at site i; n_i is the particle-number operator. This effective Hamiltonian is restricted to the Hilbert subspace with one or less electrons on each site, and the constraint of no doubly occupied site is ensured by the definition of the $d_{i\sigma}$ fermion operators. The parameters t and J describe the hopping matrix element and the Heisenberg coupling between nearest-neighbor sites. The main results on the t-J model have been obtained either from mean-field-type[7-11] or numerical[12-14] calculations. In this work a self-consistent cluster approach, based on the Caron-Pratt approximation,[15-20] is applied to investigate the magnetic and metallic properties of high-T_c materials. The simple cluster calculations are performed to examine the phase diagram of the t-J model and the dependence of the antiferromagnetic and metallic order parameters on the doping concentration and temperature.

II. CARON-PRATT APPROXIMATION

In order to examine the antiferromagnetic properties of the CuO_2 planes, we decompose the square lattice into two sublattices A and B in such a way that all neighbors of a site from sublattice A belong to sublattice B and vice versa. We propose to use a generalized cluster Caron-Pratt approximation[15-20] to obtain the metallic and magnetic phase diagrams for the t-J model. In this approach we take into account a one-site cluster and self-consistently couple the cluster to its environment by considering the surroundings as a particle reservoir which can exchange electrons with the cluster. The hopping between the cluster and immediate neighborhood is replaced by fermion source terms, which can create or annihilate electrons in the cluster. Namely, we replace the kinetic term in the Hamiltonian $-t\sum_j d_{i\sigma}^{\dagger}d_{j\sigma}$ by $-zt(d_{i\sigma}^{\dagger}\langle d_\sigma\rangle^{A(B)}+\text{H.c.})$, where (i,j) are the nearest neighbors and z is the coordination number. $\langle\cdots\rangle^{A(B)}$ denotes the thermal average for the sublattice A (B). If site i belongs to sublattice A, all its nearest neighbors belong to sublattice B and the thermal averages are calculated for sublattice B and vice versa.[20] The superexchange interaction and correct energy associated with the charge fluctuations are treated in the mean-field approximation with the same self-consistency condition as in the kinetic term [replacing $\sum_j(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_in_j)$ by $z(S_i^z\langle S^z\rangle^{A(B)}-\frac{1}{4}n_i\langle n\rangle^{A(B)})$]. Then the resulting Hamiltonian becomes a sum of one-site Hamiltonians,

$$H=\sum_{i=1}^{N}H_i^{A(B)}\ , \tag{2}$$

with

$$H_i^{A(B)}=-zt\sum_\sigma[d_{i\sigma}^{\dagger}\langle d_\sigma\rangle^{B(A)}+(\langle d_\sigma\rangle^{*})^{B(A)}d_{i\sigma}]$$
$$+zJ(S_i^z\langle S^z\rangle^{B(A)}-\tfrac{1}{4}n_i\langle n\rangle^{B(A)}-\mu n_i)\ , \tag{3}$$

where N is the number of sites. The sublattice index (A or B) depends on which sublattice site i belongs to. Under the assumption that each atom in the environment behaves in the same way as the one we are looking at (within the framework of a given sublattice), the averages $\langle\cdots\rangle^{A(B)}$ can be calculated as expected values of the operators in the site i (for i belongs to sublattice A or B, respectively), $\langle O\rangle^{A(B)}=\langle O_i\rangle$ for $O_i=d_{i\sigma},d_{i\sigma}^{\dagger},S_i^z,n_i$, where

$$\langle O_i\rangle=\frac{\mathrm{Tr}[\exp(-\beta H)O_i]}{\mathrm{Tr}\exp(-\beta H)}\ , \tag{4}$$

$\beta=1/k_BT$, k_B is the Boltzmann constant, and the Hamiltonian H is given by (2). The anticommutation properties of the operators $d_{i\sigma}$ and $d_{j\sigma'}^{\dagger}$ imply that the averages $\langle d_{i\sigma}\rangle$ and $\langle d_{j\sigma'}^{\dagger}\rangle$ cannot be simple c-numbers, but they must obey

$$\{d_{i\sigma},d_{j\sigma'}^{\dagger}\}=\{\langle d_{i\sigma}\rangle,d_{j\sigma'}^{\dagger}\}$$
$$=\{d_{i\sigma},\langle d_{j\sigma'}^{\dagger}\rangle\}=\{\langle d_{i\sigma}\rangle,\langle d_{j\sigma'}^{\dagger}\rangle\}=0\ ,$$

for $i\neq j$ or $\sigma\neq\sigma'$.[21–23] The same relations must be satisfied by averages of pairs of the operators $d_{i\sigma},d_{j\sigma'}$ and $d_{i\sigma}^{\dagger},d_{j\sigma'}^{\dagger}$. A similar situation occurs in quantum field theory, where the Grassmann numbers are used to describe fermion sources. The one-site Hamiltonians (3) consist of an even number of fermion operators and fermionlike numbers and thus commute at different sites. For instance,

$$[d_{i\sigma}^{\dagger}\langle d_{i\sigma}\rangle,d_{j\sigma'}^{\dagger}\langle d_{j\sigma'}\rangle]=d_{i\sigma}^{\dagger}\{\langle d_{i\sigma}\rangle,d_{j\sigma'}^{\dagger}\}\langle d_{j\sigma'}\rangle-d_{i\sigma}^{\dagger}d_{j\sigma'}^{\dagger}\{\langle d_{i\sigma}\rangle,\langle d_{j\sigma'}\rangle\}$$
$$+\{d_{i\sigma}^{\dagger},d_{j\sigma'}^{\dagger}\}\langle d_{i\sigma}\rangle\langle d_{j\sigma'}\rangle-d_{j\sigma'}^{\dagger}\{d_{i\sigma}^{\dagger},\langle d_{j\sigma'}\rangle\}\langle d_{i\sigma}\rangle=0\ ,$$

for $i\neq j$.

Since the Hamiltonian (2) is a sum of commuting terms, expression (4) can be simplified and the averages can be calculated self-consistently with respect to the one-site Hamiltonian (3):

$$\langle O_i\rangle=\frac{\mathrm{Tr}[\exp(-\beta H^{A\,(B)})O_i]}{\mathrm{Tr}\exp(-\beta H^{A\,(B)})}\ . \tag{5}$$

If the site i belongs to sublattice A, the average has to be calculated with the Hamiltonian H^B and vice versa.

The Hamiltonian (3) operates in a Hilbert space without states of doubly occupied sites, spanned by the basic vectors

$$|1\rangle=|\Theta\rangle\ ,\quad |2\rangle=d_{i\uparrow}^{\dagger}|\Theta\rangle\ ,\quad |3\rangle=d_{i\downarrow}^{\dagger}|\Theta\rangle\ , \tag{6}$$

where $|\Theta\rangle$ is a state without electrons in ith site. On the base (6) the operators $d_{i\uparrow}^{\dagger},d_{i\downarrow}^{\dagger},S_i^z,n_i$ take the form

$$d_{i\uparrow}^{\dagger}=\begin{bmatrix}0&0&0\\1&0&0\\0&0&0\end{bmatrix},\quad d_{i\downarrow}^{\dagger}=\begin{bmatrix}0&0&0\\0&0&0\\1&0&0\end{bmatrix}.$$
$$S_i^z=\begin{bmatrix}0&0&0\\0&\frac{1}{2}&0\\0&0&-\frac{1}{2}\end{bmatrix},\quad n_i=\begin{bmatrix}0&0&0\\0&1&0\\0&0&1\end{bmatrix}, \tag{7}$$

and the Hamiltonian (3) is

$$H^{A\,(B)}=\begin{bmatrix}0&\Delta_{\uparrow}^{*B\,(A)}&\Delta_{\downarrow}^{*B\,(A)}\\\Delta_{\uparrow}^{B\,(A)}&A_{+}^{B\,(A)}&0\\\Delta_{\downarrow}^{B\,(A)}&0&A_{-}^{B\,(A)}\end{bmatrix}, \tag{8}$$

where

$$\Delta_{\sigma}^{A\,(B)}\equiv -zt\langle d_{i\sigma}\rangle^{A\,(B)}\ ,$$
$$A_{\pm}^{A\,(B)}\equiv\tfrac{1}{2}zJ(\pm\langle S_i^z\rangle^{A\,(B)}+\tfrac{1}{2}\langle n_i\rangle^{A\,(B)})-\mu\ . \tag{9}$$

Let us focus our attention on a given site from sublattice A, and so the sublattice index will be omitted. The application of the forthcoming analyses to a site from sublattice B is quite straightforward. The energy spectrum can be obtained from the secular equations

$$E^3-E^2(A_+A_-)+E(A_+A_--|\Delta_{\uparrow}|^2-|\Delta_{\downarrow}|^2)$$
$$+|\Delta_{\uparrow}|^2A_-+|\Delta_{\downarrow}|^2A_+=0\ . \tag{10}$$

The Hamiltonian (8) can be easily diagonalized, and the corresponding eigenvectors are given by

$$|\Psi_k\rangle=\alpha_k|1\rangle+\beta_k|2\rangle+\gamma_k|3\rangle\ ,\quad k=1,2,3\ , \tag{11}$$

where

$$\alpha_k=\left[1+\frac{|\Delta_{\uparrow}|^2}{(E_k-A_+)^2}+\frac{|\Delta_{\downarrow}|^2}{(E_k-A_-)^2}\right]^{-1/2}, \tag{12a}$$

$$\beta_k=\frac{\Delta_{\uparrow}}{(E_k-A_+)}\alpha_k\ , \tag{12b}$$

$$\gamma_k=\frac{\Delta_{\downarrow}}{(E_k-A_-)}\alpha_k\ , \tag{12c}$$

where E_k are the solutions of Eq. (10).

According to (7), at zero temperature we get

$$\langle d_{i\uparrow}\rangle=\alpha_1\beta_1\ ,\quad \langle d_{i\downarrow}\rangle=\alpha_1\gamma_1\ ,$$
$$\langle S_i^z\rangle=\tfrac{1}{2}(\beta_1^2-\gamma_1^2)\ ,\quad \langle n_i\rangle=\beta_1^2+\gamma_1^2\ , \tag{13}$$

where $\alpha_1,\beta_1,\gamma_1$ are calculated from Eqs. (12) with E_1 being the lowest eigenvalue of the Hamiltonian (8). It is easy to show that at half filling the ground state of the Hamiltonian (8) is antiferromagnetic. The half filling ($\langle n\rangle=1$) and normalization constraint ($\langle\Psi|\Psi\rangle=1$) gives $\alpha_1=0$, and all the "metallic" parameters[17,19,20] $\Delta_{i\sigma}$ have to be equal to zero. In this case the Hamiltonian (8) (assuming that site i belongs to the sublattice B) takes an extremely simple form:

$$H^B=\begin{bmatrix}0&0&0\\0&A_{+}^{A}&0\\0&0&A_{-}^{A}\end{bmatrix}. \tag{14}$$

Assuming $\langle S_i^z\rangle^A>0$, the lowest eigenvalue of (14) is $E_1=A_{-}^{A}$. From Eqs. (12) and (13) we obtain $\beta_1=0$, $\gamma_1=1$, and $\langle S_i^z\rangle^B=-\frac{1}{2}$. Replacing H^B with H^A in Eq. (14), we get $E_1=A_{+}^{B}$, $\beta_1=1$, $\gamma_1=0$, and $\langle S_i^z\rangle^A=\frac{1}{2}$.

At finite temperature and/or at finite doping, there exist ferro-, antiferro-, and paramagnetic solutions, and the free energy determines the nature of the ground state.

III. RESULTS AND DISCUSSIONS

The system of nonlinear equations (5), (9), (10), and (12) has been solved self-consistently for various values of n and t/J at zero and nonzero temperatures. The solutions determine the phases of the model as follows: (i) $\Delta=0$, insulating phases (I); (ii) $\Delta\neq0$, metallic phases (M); (iii) $\langle S_i^z\rangle^A=\langle S_i^z\rangle^B=0$, paramagnetic phases (PM); (iv) $\langle S_i^z\rangle^A=\langle S_i^z\rangle^B\neq0$, ferromagnetic phases (FM); and (v)

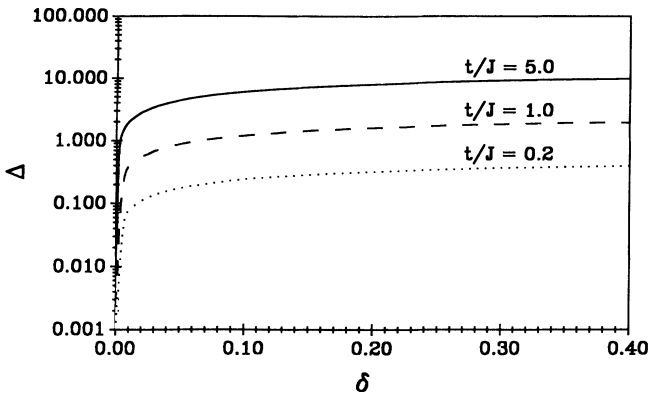

FIG. 1. Metallic order parameter Δ as a function of hole concentration δ at zero temperature for $t/J=5.0$, 1.0, and 0.2.

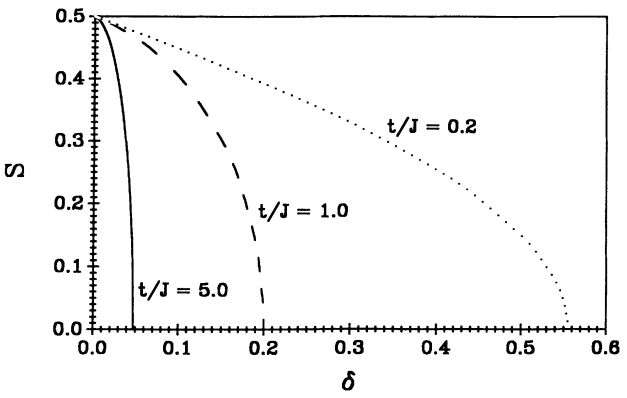

FIG. 3. AF order parameter S as a function of hole concentration δ at zero temperature for $t/J=5.0$, 1.0, and 0.2.

$\langle S_i^z\rangle^A=-\langle S_i^z\rangle^B\neq 0$, antiferromagnetic phases (AF).

The metallic order parameter Δ is defined by

$$\Delta^2=\Delta_\uparrow^2+\Delta_\downarrow^2 \ . \tag{15}$$

In the insulating region ($\Delta=0$), the model can be solved analytically giving a generalized Ising-like AF solution:

$$\langle S_i^z\rangle^A=-\langle n_i\rangle\tanh(-\beta zJ\langle S_i^z\rangle^A) \ , \tag{16}$$

$$\langle S_i^z\rangle^B=-\langle S_i^z\rangle^A \ ,$$

with the Néel temperature T_N:

$$k_B T_N=\tfrac{1}{4}\langle n_i\rangle zJ \ . \tag{17}$$

The free energy in the insulating region is given by

$$F=k_B T\ln\langle n_i\rangle \ . \tag{18}$$

In order to obtain the metallic solutions, the system of Eqs. (5), (9), (10), and (12) has been solved numerically for square lattice ($z=4$). In the case of zero doping ($n=1$), the only solution has an insulating nature; otherwise, metallic states minimize the free energy. When decreasing the doping concentration δ ($\delta\equiv 1-\langle n_i\rangle$), the metallic parameter Δ tends to zero, as is shown in Fig. 1. In the insulating region ($n=1$), a real particle motion is impossible because of the single-occupancy constraint, but a virtual hopping can occur.[16]

For each value of the ratio t/J, there is a critical doping concentration above which magnetic solutions do not exist. In the case of zero temperature, the critical value δ_c can be calculated from Eqs. (9), (10), (12), and (13):

$$\delta_c=\frac{1}{4t/J+1} \ . \tag{19}$$

Below δ_c there exist AF as well as FM solutions, but for all values of t/J the AF solution minimizes the free energy. The phase diagram is shown in Fig. 2. For $t/J=5$ the critical doping concentration $\delta_c=0.05$; this is in agreement with the results obtained by mean-field treatment[11] as well as Monte Carlo methods.[13] Figure 3 shows the AF order parameter as a function of doping concentration. The AF order parameter S is defined by

$$S=\pm\langle S_i^z\rangle \ , \tag{20}$$

where the sign depends on which sublattice site i belongs to. Increasing the number of nonoccupied sites destroys the AF order, and a second-order phase transition to the nonmagnetic state appears at the threshold point. The critical doping concentration decreases with the increase

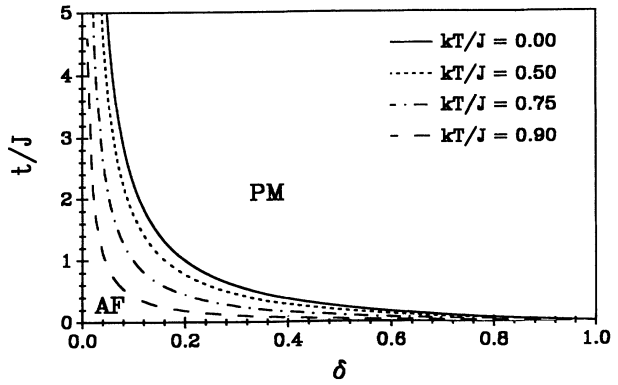

FIG. 2. Phase diagram in the plane t/J vs hole concentration δ for temperatures $kT/J=0.00$, 0.50, 0.75, and 0.90.

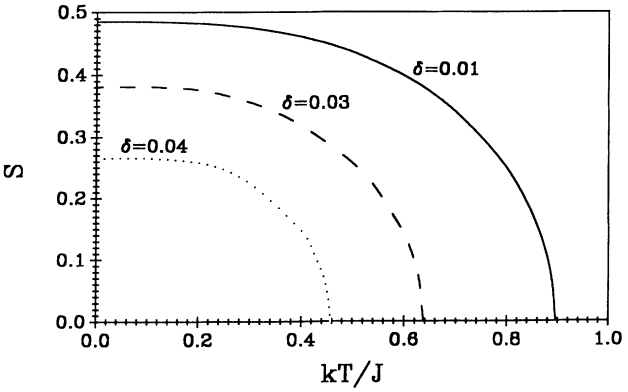

FIG. 4. Temperature dependence of the AF order parameter S for hole concentration $\delta=0.01$, 0.03, and 0.04 for $t/J=5$.

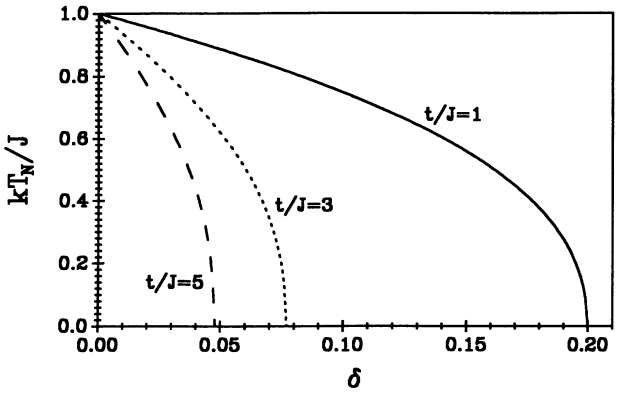

FIG. 5. Néel temperature as a function of hole concentration for $t/J = 5.0$, 3.0, and 1.0.

of the temperature of the system. The AF order parameter S versus temperature T is plotted in Fig. 4. The moment the temperature reaches the critical value (the Néel temperature), a second-order phase transition is observed. The Néel temperature is plotted as a function of the doping concentration in Fig. 5. When the doping concentration decreases, the Néel temperature tends to the value calculated from Eq. (17), approaching this value in the insulating region ($n = 1$).

The main aim of the present work was to examine the ability of the mathematically simple Caron-Pratt approach to characterize the magnetic and metallic phases of the t-J model. On the other hand, the simplicity of this approximation is obtained by neglecting many important effects: The analyses were performed at the mean-field level, losing local spin and charge fluctuations and the lattice topology, and therefore details of the electronic spectrum were lost. The present approach is not applicable to describing superconducting states. This approximation may be improved by taking into account larger clusters, for which not only I, M, FM, AF, and PM, but also resonating-valence-bond,[2] flux,[9,24] chiral,[25] or dimer[26] phases could be defined.

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