Nonplanar spiral states of the t-J model with classical spins

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The spiral state in the two-dimensional t-J model is studied by numerical diagonalization of an effective Hamiltonian. We examine all possibilities of the spiral spin states including the nonplanar states. It is found that nonplanar spiral states occur, but the deviations from the planar spiral state in the nonplanar spiral states are small for small hole concentrations where our effective Hamiltonian is valid. The modulation of the spin configuration increases continuously from the antiferromagnetic order as the hole concentration increases, and discontinuously changes at a critical hole concentration. Then the state undergoes the first-order phase transition either to the $(\pi, 0)$ phase or to the ferromagnetic phase, depending on the value of J/t.

I. INTRODUCTION

The doped antiferromagnet on a square lattice is a remarkably interesting topic especially in connection with high-temperature superconductivity. The t-J model is one of the models studied extensively in this context. In the case of half-filling, this model becomes an $S=1/2$ antiferromagnetic Heisenberg model, which is believed to have a Néel ordered ground state. Then what state becomes the ground state when holes are doped in this system? Nagaoka proved that if a single hole is doped into the half-filled band, the ground state of the Hubbard model with $U = \infty$, i.e., the t-J model with $J = 0$, is the ferromagnetic state with the maximum total spin to gain the maximum kinetic energy.[1] Putikka *et al.* argued that this ferromagnetic state extends up to a finite hole concentration.[2]

On the other hand, when both the exchange coupling and the hole concentration are finite, the t term and the J term compete with each other. The exchange interaction favors antiferromagnetic order, while motions of the holes tend to destroy this order.[3] The spin spiral state proposed by Shraiman and Siggia is a candidate for the ground state in this region.[4] Their approach is based on the nonlinear σ model that describes the low-energy, long-wavelength behavior of the t-J model. Since the spiral spin configuration is modulated from rigid Néel order (see Fig. 1), holes can hop more freely than in the classical Néel ordered background. Several groups showed within the slave-fermion mean field approximation that the spiral state has the lowest energy.[5–7] We have obtained similar results with a more physically transparent technique.[10] In those analyses, the direction of each spin is assumed to be confined in a plane; i.e., only the planar spiral states are assumed. However, there is no justification for this simplification. We take into account nonplanar spiral order in this paper and examine the validity of the assumption of the planar spiral.

This paper is organized as follows. In Sec. II, we simplify the Hamiltonian by a classical approximation of the spin degrees of freedom. This is different from the ordinary slave-particle techniques and a clearer discussion can be done on the interplay between spins and charges. In Sec. III, we calculate the ground state energy of this approximate Hamiltonian for various spiral modulations by diagonalizing the simplified Hamiltonian numerically. We can treat much larger systems for this Hamiltonian than for the original Hamiltonian. Taking into account all possible spiral states and searching the lowest-energy state, we determine the phase diagram.

We shall work in units such that $\hbar = 1$ and the lattice constant $a = 1$.

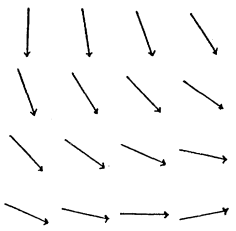

FIG. 1. A schematic picture of a planar spiral state $[\mathbf{q}_1 = (0,0), \mathbf{q}_2 = (q_x, q_y)]$.

II. CLASSICAL SPIN APPROXIMATION

The t-J Hamiltonian is defined as

$$H = -t \sum_{\langle i,j\rangle,\sigma} (\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + \text{H.c.}) + J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

$$\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i-\sigma}), \tag{2}$$

where $c_{i\sigma}$ represents the annihilation operator of an electron at the ith site with spin σ ($\sigma = \pm 1$) and $n_{i\sigma} \equiv c^{\dagger}_{i\sigma}c_{i\sigma}$. A spin operator is defined by $S^l_i = \frac{1}{2}\sum_{\sigma\tau} c^{\dagger}_{i\sigma}\sigma^l_{\sigma\tau}c_{i\tau}$ where σ^l is the lth component of the Pauli spin matrix ($l = x, y, z$). The first term describes the electron hopping with double occupancy excluded and the second represents the antiferromagnetic exchange interaction ($J > 0$).

When we study the t-J model, we take a viewpoint that the model is only an effective one derived from a more realistic model with an assumption of the absence of the long-range part of the Coulomb interaction. Thus, for example, when we consider inhomogeneous charge distributions in a macroscopic spatial scale, we have to be careful about that such inhomogeneous charges would not be screened sufficiently that the Coulomb interactions become short range as in the t-J model. Since such long-range Coulomb interactions would raise the total energy, such inhomogeneous states would not occur in realistic models. Therefore, we study the model under the assumption of the absence of such inhomogeneous charge distributions as many authors have done so far.

Our formulation is the same as that of a previous paper[10] except that we retain all possible spin configurations. The following identities relate the operator $\tilde{c}_i$ and $\mathbf{S}_i$:

$$\begin{aligned} &\tilde{c}_{i\sigma} = c_{i-\sigma}S^{-\sigma}_i, \\ &\tfrac{1}{2}\sigma\tilde{c}_{i\sigma} = c_{i\sigma}S^z_i, \\ &0 = c_{i\sigma}S^{-\sigma}_i. \end{aligned} \tag{3}$$

Using Eq. (3), we write the Hamiltonian in the form

$$H = -\frac{4}{3}t \sum_{\langle i,j\rangle,\sigma} (\mathbf{S}_i c^{\dagger}_{i\sigma}c_{j\sigma}\mathbf{S}_j + \text{H.c.}) + J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{4}$$

This form of the Hamiltonian transparently describes how electrons move on the lattice disturbing the surrounding spins. A similar form was studied by Xu *et al.*[9]

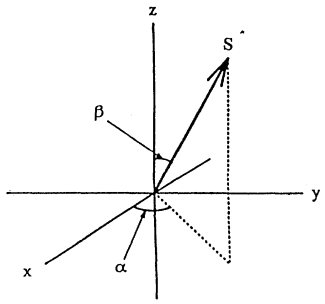

FIG. 2. The azimuthal angle α and the polar angle β of a classical spin.

We introduce a rotated spin coordinate on every site for convenience. We rotate the coordinate about the z axis by an angle α_i and successively about the y axis by β_i at the ith site (see Fig. 2). By these rotations, the spin $\mathbf{S}$ and the two-component spinor $\mathbf{c}^{\dagger}_i = (c^{\dagger}_{i\uparrow}\ c^{\dagger}_{i\downarrow})$ are transformed into

$$\mathbf{S}'_i \equiv U_i\mathbf{S}_i, \quad \mathbf{d}_i \equiv \begin{pmatrix} d_{i\uparrow} \\ d_{i\downarrow} \end{pmatrix} = R_i\mathbf{c}_i, \tag{5}$$

where

$$U_i = \begin{pmatrix} \cos\beta_i & 0 & -\sin\beta_i \\ 0 & 1 & 0 \\ \sin\beta_i & 0 & \cos\beta_i \end{pmatrix} \begin{pmatrix} \cos\alpha_i & \sin\alpha_i & 0 \\ -\sin\alpha_i & \cos\alpha_i & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{6}$$

$$R_i = \begin{pmatrix} e^{-i\alpha_i/2}\cos\frac{\beta_i}{2} & -e^{-i\alpha_i/2}\sin\frac{\beta_i}{2} \\ e^{i\alpha_i/2}\sin\frac{\beta_i}{2} & e^{i\alpha_i/2}\cos\frac{\beta_i}{2} \end{pmatrix}. \tag{7}$$

We apply the classical spin approximation; i.e., we treat a spin operator $\mathbf{S}_i$ as a c number. Now, we assume that the spin system has some order in the ground state. We adjust the z axis to the direction of the spin at each site, so that all spins are ferromagnetically ordered in the new coordinates. Thus, the ground state is the vacuum state with respect to $d_{i\downarrow}$'s. Further, creations of $d^{\dagger}_{i\downarrow}$ are prohibited by the local constraint due to the infinite Coulomb repulsion. Therefore operations of $d_{i\downarrow}$'s and $d^{\dagger}_{i\downarrow}$'s to the state should lead to zero. Hence we omit $d_{i\downarrow}$ and write d_i instead of $d_{i\uparrow}$ from now on. Any spin configuration can be characterized by the variables $\{\alpha_i\}$ and $\{\beta_i\}$. By this classical spin approximation, the hopping term and exchange term are transformed into

$$H_t = -\frac{4}{3}tS^2 \sum_{\langle i,j\rangle} \left(e^{i(\alpha_i-\alpha_j)/2}\cos\frac{\beta_i}{2}\cos\frac{\beta_j}{2} + e^{-i(\alpha_i-\alpha_j)/2}\sin\frac{\beta_i}{2}\sin\frac{\beta_j}{2} \right) [\cos(\alpha_i - \alpha_j)\sin\beta_i\sin\beta_j + \cos\beta_i\cos\beta_j] d^{\dagger}_i d_j, \tag{8}$$

$$H_J = JS^2 \sum_{\langle i,j\rangle} [\cos(\alpha_i - \alpha_j)\sin\beta_i\sin\beta_j + \cos\beta_i\cos\beta_j]. \tag{9}$$

Thus, our problem is reduced to solving the eigenvalue equation of an $N \times N$ matrix, when the spin configuration is fixed. Here N is the number of sites.

For the half-filled case, there is no contribution from the t term because of the Pauli principle. Thus the ground state has Néel order for the half-filled band because it has the minimum exchange energy. In the following sections, we consider the situations where the hole concentration deviates from half-filling.

III. SPIN SPIRAL STATE

Now, we consider the spin spiral state where the spins are systematically rotating. A spiral pattern is characterized by a set of two vectors $\mathbf{q}_1$ and $\mathbf{q}_2$, which specify the wave number of the modulation measured from the ferromagnetic configuration of spins. The azimuthal and polar angles of the direction of the classical spin at the ith site, α_i and β_i, are given by

$$\alpha_i = \mathbf{q}_1 \cdot \mathbf{r}_i, \qquad \beta_i = \mathbf{q}_2 \cdot \mathbf{r}_i \tag{10}$$

for spiral states, where $\mathbf{r}_i$ is the lattice vector associated with the site i. With this definition, the ferromagnetic state corresponds to $\mathbf{q}_1 = (0,0)$ and $\mathbf{q}_2 = (0,0)$ and the Néel state corresponds to $\mathbf{q}_1 = (0,0)$ and $\mathbf{q}_2 = (\pi,\pi)$. For planar spiral phases where $\mathbf{q}_1 = (0,0)$, we can easily diagonalize the Hamiltonian by Fourier transformation. In our previous paper,[10] we analyzed this model in the low doping regime, assuming that only the diagonal spiral phases [$\mathbf{q}_1 = (0,0)$ and $\mathbf{q}_2 = (q,q)$] and the stripe spiral phases [$\mathbf{q}_1 = (0,0)$ and $\mathbf{q}_2 = (\pi,q)$] are possible. We have found that the diagonal spiral state always gives a lower energy than the stripe spiral state at the same parameter and that the deviation of its spiral pitch from $\mathbf{q}_1 = (0,0), \mathbf{q}_2 = (\pi,\pi)$ is almost proportional to the hole concentration. There, we have also found a first-order phase transition from the diagonal spiral state to the ferromagnetic state at some critical hole concentration.

In our present study we solve the effective Hamiltonian (8) on finite lattices to investigate more general spiral patterns. For the $L \times L$ lattice ($L^2 = N$), $(\mathbf{q}_1, \mathbf{q}_2)$ can only take $(2\pi n/L, 2\pi m/L)$ (n, m are integers) in the periodic boundary condition. The number of essentially different sets of $(\mathbf{q}_1, \mathbf{q}_2)$ is about $N^2/16$ if we take the symmetry of the square lattice into account. We diagonalize the Hamiltonian (8) numerically for all possible $\mathbf{q}_1, \mathbf{q}_2$ for $L = 12, 16, 20$ and determine the optimum spiral pitch. In what follows, we show the phase diagrams up to $\delta = 0.35$. This value of δ is only for convenience, and does not indicate the limit of δ below which our theory is valid.

The spiral pitches that minimize the energy are shown in Fig. 3 for various doping concentrations δ and J/t. We can see from this figure that the spiral state gives the lowest energy in the lightly doped region for fixed J. The nonplanar spiral phase is obtained in the more heavily doped region. Their pitches $|\mathbf{q}_1|, |\mathbf{q}_2|$ increase with δ and decrease with J/t.

We find a phase transition from the spiral state to the ferromagnetic state at a small J/t. This transition is consistent with the analytic result in the low doping region.[10] Besides this, we also find a transition from the spiral state to the state with the spiral pitches $\mathbf{q}_1 = \mathbf{0}, \mathbf{q}_2 = (\pi,0)$ for larger J/t. We call this phase the $(\pi,0)$ state. These two transitions seem to be discontinuous, although our resolution is limited by the lattice size. The $(\pi,0)$ state was not found by our previous analysis in the low doping region because this needs rather higher doping than the ferromagnetic state. This situation will be clarified by the following discussion. We compare the kinetic energies of systems in the ferromagnetic state and the $(\pi,0)$

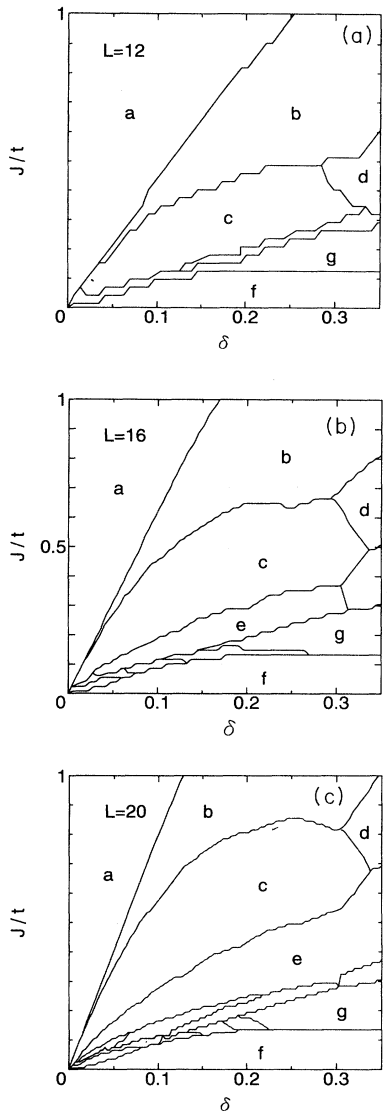

FIG. 3. Phase diagrams in the ground state for 12×12, 16×16, and 20×20 lattices. (a) $\mathbf{q}_1$=$(0,0)$, $\mathbf{q}_2$=(π,π); (b) $\mathbf{q}_1$=$(0,0)$, $\mathbf{q}_2$=$(\pi,\pi - 2\pi/L)$; (c) $\mathbf{q}_1$=$(0,0)$, $\mathbf{q}_2$=$(\pi-2\pi/L,\pi-2\pi/L)$; (d) $\mathbf{q}_1$=$(2\pi/L,0)$, $\mathbf{q}_2$=$(\pi,\pi-2\pi/L)$; (e) $\mathbf{q}_1$=$(2\pi/L,2\pi/L)$, $\mathbf{q}_2 = (\pi - 2\pi/L,\pi - 2\pi/L)$; (f) $\mathbf{q}_1$=$(0,0)$, $\mathbf{q}_2$=$(0,0)$ (ferromagnetic state); (g) $\mathbf{q}_1$=$(0,0)$, $\mathbf{q}_2$=$(\pi,0)$ [$(\pi,0)$ state].

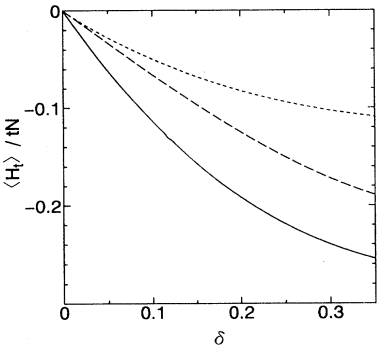

FIG. 4. Kinetic energy plotted versus hole concentration. The solid, dotted, and dashed lines correspond to the ferromagnetic, spin-disordered, and $(\pi, 0)$ states, respectively.

state for various hole concentrations in Fig. 4. Since the ferromagnetic state has the lower kinetic energy than the $(\pi, 0)$ state, the small J/t region is occupied by the ferromagnetic state. On the other hand, for large J/t, the ferromagnetic state is disadvantageous due to the exchange term and thus the $(\pi, 0)$ state is favored. However, the $(\pi, 0)$ state does not appear for small hole concentrations because the spiral state is energetically favored there.

It is found from Fig. 3 that the areas of the ferromagnetic state and the $(\pi, 0)$ state are almost independent of the lattice sizes. Thus, we expect that the areas remain almost the same in the thermodynamic limit. On the other hand, the region of the spiral state changes with the lattice size. In particular, the area of the nonplanar spiral phase seems to expand with the lattice size. In the thermodynamic limit, this area should be larger, although we cannot say whether it extends to the zero hole concentration. For the spiral phase, the system size dependence appears to be strong in the phase diagram. However, this is due to the discreteness of $\mathbf{q}_1$ and $\mathbf{q}_2$: Spiral states with spiral pitches smaller than $2\pi/L$ do not occur in the finite-size system of $L \times L$. If we take into account this discreteness, we can see that our results show a tendency of convergence, as in Fig. 5. Figures 5(a) and 5(b) are for $\delta = 0.031\,25$ and Figs. 5(c) and 5(d) are for $\delta = 0.25$. The same tendency is seen for the other hole concentrations.

IV. SUMMARY AND DISCUSSION

We have analyzed the t-J model assuming that there is a static magnetic structure in its ground state. As we mentioned in the Introduction, most theories on the spiral state assume the planar spiral modulation *a priori* without justification. We have confirmed that the deviation from the planar spiral modulation is small for small hole densities. Besides our analyses suggest that nonplanar modulations are likely to appear, especially for moderate hole densities. Kane and co-workers proposed the possibility of a nonplanar spiral state called the "double spiral state" where spins spiral in orthogonal planes in the x and y directions.[11,12] This is one of the nonplanar spiral states which correspond to the case $\mathbf{q}_1 = (q, 0), \mathbf{q}_2 = (0, q)$. They concluded that this double spiral state has a higher mean field energy than planar spiral states. This double spiral state does not appear also in our phase diagram, but we found other nonplanar spiral states in our phase diagram.

If the concentration of holes increases, a ferromag-

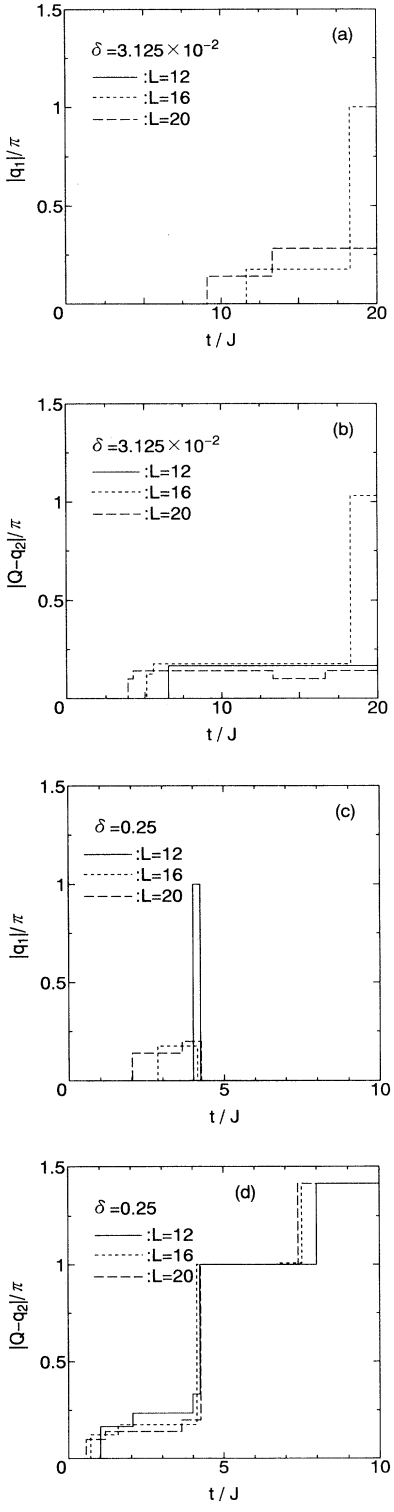

FIG. 5. Deviations from the Néel order plotted versus t/J.

netic or $(\pi, 0)$ ground state appears instead of the spiral state. There have been reported similar results concerning the incommensurate antiferromagnetic orders for the Hubbard model.[13,14] These theories also predicted the transition from the diagonal spiral state to the ferromagnetic state. But the transition between the ferromagnetic phase and the spiral phase in the theories is second order in contrast to the first-order transition in our case. We show in Fig. 6 a schematic phase diagram expected in the thermodynamic limit.

Here, we examine the spin-disordered state. Vignale examined the spin-disordered state, which is characterized by a static random spin density in the Hubbard model using the Hartree-Fock approximation.[8] We estimate the energy of the spin-disordered state to examine whether it has lower energy than other ordered states. We generate the disordered configurations of spins by uniform random numbers. We calculate the kinetic energy for each spin configuration and average them over various random configurations. In Fig. 4, the kinetic energy of the spin-disordered state and that of the $(\pi, 0)$ state are shown. This calculation has been done for a 16×16 lattice and the number of averaged samples is 1280. These kinetic energies are equal to the total energy for both states, because they have zero total exchange energy. From Fig. 4, we conclude that the $(\pi, 0)$ state is more favored for all hole concentrations than the spin-disordered state. Thus, the spin-disordered state without spin correlations does not appear in our phase diagram.

Although we did not consider the charge fluctuation effect, the stability of the spiral state against charge fluctuations has been studied in several papers.[6,7,10] Emery *et al.* pointed out the possibility of phase separation between the hole-rich region and the hole-poor region.[15] The physical reason for phase separation is that the gain in exchange energy by maximizing the number of antiferromagnetic bonds outweighs the cost in kinetic energy. The phase separation occurs also in our approximation, unless we ignore its possibility, as we examined in our previous paper.[10] However, we have ignored such a state in this paper assuming that the long-range part of the Coulomb interaction prohibits holes from the phase separation, since we are interested in the spiral states which might exist in real materials such as high-T_c cuprates.

The main approximation employed to obtain the above results is the classical treatment of spins. We have fixed the magnitudes of spins on each site regardless of the doping of holes. This approximation violates the local constraint for the number of holes at each site. This would be very harmful except for small hole concentrations, which we are interested in. We can partly take into account the shrinkage of spins due to this constraint

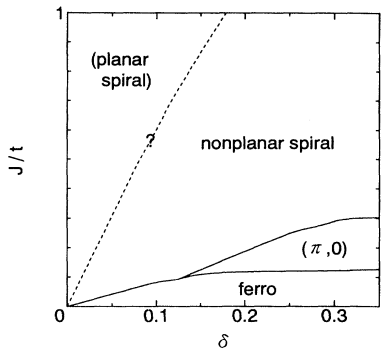

FIG. 6. A schematic phase diagram of the classical spin t-J model expected in the thermodynamic limit.

by the substitution $\mathbf{S}_i \rightarrow (1 - \delta/2S)\mathbf{S}_i$, assuming they are uniform. Because both H_t and H_J become smaller by the same factor of $(1 - \delta/2S)^2$, this makes no change in our phase diagrams. There are correlations between the shrinked spins and doped holes in actuality, because they have the same degrees of freedom originally. Thus the spin shrinkages are not uniform and fluctuations exist. The effects of such fluctuations become serious for high hole densities. The large values of δ in our phase diagrams might be out of the range in which our approximation is valid. For example, if fluctuations are taken into account, the ordered states would disappear at a critical hole concentration. In particular, if we take only the antiferromagnetic order into account, the magnetic order disappears at a critical hole concentration.[3,16] However, in the large S limit, the fluctuations would be negligible. Our approximation corresponds to taking the leading order of a Holstein-Primakoff-type spin wave expansion. We have argued the effect of spin wave scattering in our previous paper.[10] Calculations of higher-order corrections are further complex problems.

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