Spiral spin states in a generalized Kondo lattice model with classical localized spins

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(Received 13 September 1994; revised manuscript received 4 October 1994)

A generalized Kondo lattice model with classical localized spins is studied in a two-dimensional case. Our model includes the case in which antiferromagnetic exchange coupling J exists between localized spins. We obtain the magnetic phase diagram on the plane of J and fermion concentration n, and the order of each phase transition on the phase diagram, taking into account all possible planar spiral orders and canted ferromagnetic orders as well as the Néel order and the ordinary ferromagnetic order. In the phase diagram, we find a large region of the stripe spiral phase, which is consistent with the results of neutron-scattering experiments of $La_{2-x}Sr_xCuO_4$.

Models of mobile fermions and localized spins have attracted much attention in connection with the heavy-fermion compounds and the copper oxide high-temperature superconductors.[1-6] We define the spin-fermion model on the square lattice by

$$H=H_0+H_K\ , \tag{1}$$

$$\begin{aligned} H_0&=H_t+H_J\ ,\\ H_t&=-t\sum_{(i,j),\sigma}(p^\dagger_{i\sigma}p_{j\sigma}+\text{h.c.})-\mu\sum_{i,\sigma}p^\dagger_{i\sigma}p_{i\sigma}\ ,\\ H_J&=\sum_{(i,j)}J\mathbf{S}_i\cdot\mathbf{S}_j\ ,\\ H_K&=\frac{1}{2}\sum_i\sum_{\sigma_1,\sigma_2}J_K\mathbf{S}_i\cdot(p^\dagger_{i,\sigma_1}\boldsymbol{\sigma}_{\sigma_1\sigma_2}p_{i,\sigma_2})\ , \end{aligned} \tag{2}$$

where $p_{i\sigma}$ is the fermion operator on the site i with spin σ, $\mathbf{S}_i$ is the localized spin on the site i, and $\boldsymbol{\sigma}_{\sigma_1\sigma_2}$ is the (σ_1,σ_2) element of the Pauli matrix. This model is called a generalized Kondo lattice model. In the limit of $J_K=0$ or $n=0$, the model reduces to the antiferromagnetic (AF) Heisenberg model,[7] in which AF order is considered to exist at $T=0$. On the other hand in the limit of $J=0$, fermion kinetic energy stabilizes the ferromagnetic state:[3] Such effective ferromagnetic interactions are called the double exchange interactions. Therefore, a competition occurs between AF exchange interactions J and fermion kinetic energies. Such frustrations may lead to spiral-spin-ordered states as well as canted ferromagnetic (CF) states.[8-14] Further, the possibility of a spiral state has been pointed out from experiments of the copper oxides.[15] Thus, since the spin-fermion model is an appropriate model at least for a low-doping region of the copper oxides,[4] those experimental results give rise to much interest in the study of spiral states in the present model as well as the Néel state and the ferromagnetic states.

The purpose of this paper is to construct the magnetic phase diagram on the J-n plane for the whole range of n at the zero temperature, which may have areas of the spiral phases and the CF phase. For this purpose we take the classical limit of localized spins: We regard the localized spins $\mathbf{S}$ as classical variables with the magnitude S. Spin-wave corrections and shrinkage of spins due to quantum fluctuations are left for future studies. This is a good approximation for real compounds with large localized spins. The formulation in this paper is similar to that of our previous theory for the t-J model.[8,9] However, the present model is very different from the t-J model in that the spins $\mathbf{S}_i$ and the fermions $p_{i\sigma}$ have different degrees of freedom by definition. Thus we can straightforwardly take the classical spin limit only for the localized spins without touching the mobile fermions. Hence, our theory does not have any limitations on the fermion concentration for its applicability. Moreover, we can take the t-J limit, $J_K\to\infty$, in the present model, in which the spin-fermion model reduces to the t-J model. Once we introduce the classical-spin approximation of the localized spins, we can solve the problem without any further drastic approximation.

If we fix the configuration of these classical spins, our Hamiltonian is bilinear in fermion operators, which is easy to examine. We express the direction of the localized spin at each site by polar coordinates α_i,β_i as $\mathbf{S}_i=S(\sin\beta_i\cos\alpha_i,\sin\beta_i\sin\alpha_i,\cos\beta_i)$. We rotate the spin coordinate so that each spin points in the direction of the new local z axis: $\mathbf{S}_i=(0,0,S)$ in the new coordinate. Then the fermion doublet $(p^\dagger_{i\uparrow},p^\dagger_{i\downarrow})$ is also locally transformed by

$$P_i\equiv\exp(-i\alpha_i\sigma_z/2)\exp(-i\beta_i\sigma_y/2)$$

as

$$\begin{bmatrix}c_{i\uparrow}\\ c_{i\downarrow}\end{bmatrix}\equiv P_i^\dagger\begin{bmatrix}p_{i\uparrow}\\ p_{i\downarrow}\end{bmatrix}\ , \tag{3}$$

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which leads to

$$H_K=\tfrac{1}{2}J_K S\sum_i (c_{i\uparrow}^\dagger c_{i\uparrow}-c_{i\downarrow}^\dagger c_{i\downarrow}) .$$

In general, spiral states are specified by spiral wave vectors $\mathbf{q}'$ and $\mathbf{q}$ defined by $\alpha_i=\mathbf{q}'\cdot\mathbf{R}_i+\alpha_0$, and $\beta_i=\mathbf{q}\cdot\mathbf{R}_i+\beta_0$, where $\mathbf{R}_i$ is the vector to the site i in the real space, and α_0 and β_0 are constant. Then all possible spin-ordered states can be specified by $\mathbf{q}'$ and $\mathbf{q}$ in the first Brillouin zone, and α_0 and β_0. For spiral states, we only consider the states with constant α_i independent of the site i, i.e., $\mathbf{q}'=0$ for simplicity, which are called planar spiral states. We also consider the CF states, which are specified as $\mathbf{q}=0$, $\mathbf{q}'=(\pi,\pi)$, and $\beta_0\neq 0$. In this paper we examine all possible planar spiral states and CF states. The spin-disordered state is apparently of high energy in our classical-spin model. The state with $q_x=q_y$ is called the diagonal state, and that with $q_x\neq q_y$ is called the stripe state. For the spiral states, the Hamiltonian is diagonalized as

$$H=\sum_{\mathbf{k}}(\epsilon^{(+)}(\mathbf{k},\mathbf{q})d_{\mathbf{k}+}^\dagger d_{\mathbf{k}+}+\epsilon^{(-)}(\mathbf{k},\mathbf{q})d_{\mathbf{k}-}^\dagger d_{\mathbf{k}-}) +JS^2N(\cos q_x+\cos q_y) \tag{4}$$

by a unitary transformation:

$$\begin{bmatrix} d_{\mathbf{k}+} \\ d_{\mathbf{k}-} \end{bmatrix} \equiv \frac{1}{\sqrt{2D(\mathbf{k},\mathbf{q})[D(\mathbf{k},\mathbf{q})-h_3]}} \begin{bmatrix} \xi_2 & -i[D(\mathbf{k},\mathbf{q})-h_3] \\ -i[D(\mathbf{k},\mathbf{q})-h_3] & \xi_2 \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \end{bmatrix} , \tag{5}$$

where

$$\epsilon^{(\pm)}(\mathbf{k},\mathbf{q})=\xi_0(\mathbf{k},\mathbf{q})\pm D(\mathbf{k},\mathbf{q}) ,$$

$$D(\mathbf{k},\mathbf{q})=\sqrt{\{\xi_2(\mathbf{k},\mathbf{q})\}^2+(h_3)^2} ,$$

$$\xi_0(\mathbf{k},\mathbf{q})=-2t\left[\cos k_x\cos\frac{q_x}{2}+\cos k_y\cos\frac{q_y}{2}\right] , \tag{6}$$

$$\xi_2(\mathbf{k},\mathbf{q})=-2t\left[\sin k_x\sin\frac{q_x}{2}+\sin k_y\sin\frac{q_y}{2}\right] ,$$

$$h_3=J_K S/2 .$$

We take the lattice constant as unity in this paper. Thus the total energy is estimated as

$$E_{\text{spiral}}(\mathbf{q})=\sum_{\mathbf{k},s=\pm}\epsilon^{(s)}(\mathbf{k},\mathbf{q})\theta(\mu-\epsilon^{(s)}(\mathbf{k},\mathbf{q})) +JS^2N(\cos q_x+\cos q_y) . \tag{7}$$

Here, μ is the chemical potential. For CF states, the Hamiltonian is also easily diagonalized, and the total energy is obtained as

$$E_{\text{CF}}(\beta_0)=\sum_{\mathbf{k},s=\pm}\epsilon_{\text{CF}}^{(s)}(\mathbf{k},\beta_0)\theta(\mu-\epsilon_{\text{CF}}^{(s)}(\mathbf{k},\beta_0)) +2JS^2N\cos 2\beta_0 , \tag{8}$$

with

$$\epsilon_{\text{CF}}^{(s)}(\mathbf{k},\beta_0)=s\sqrt{[\epsilon(\mathbf{k})+h_3\cos\beta_0]^2+h_3\sin^2\beta_0} , \tag{9}$$

where $\epsilon(\mathbf{k})=-2t(\cos k_x+\cos k_y)$.

It is easy to obtain the total energy of the system for a given spin configuration with the above expressions. The spin configuration in the ground state is obtained by minimizing the total energy. We may directly calculate the total energy in the thermodynamic limit with sufficient accuracy by replacing the summation with an appropriate integration in the above expressions and carrying out the integration. However, we deal with sufficiently large finite-size systems in this paper, such as $L\times L$ with $L=128,256,512$ for convenience. We also discretize the canting angle β_0 as $\beta_0=\pi l/2L$, with $l=0,1,2,\ldots,L$.

Figures 1 and 2 are the phase diagrams in the ground state, for $J_K=8t/S$ and for $J_K=2t/S$, respectively. The phase boundaries for the two system sizes coincide very well as we see in Figs. 1 and 2. This indicates that our system sizes are sufficiently large for practical purposes, and the phase diagrams can be regarded as being in the thermodynamic limit. The ferromagnetic state is due to the double exchange mechanism, which at $J/t=0$ has been studied by Sigrist *et al.*[3] In the ferromagnetic phase, the total fermion kinetic energy is minimum, while the total AF exchange energy of the localized spins is maximum. The diagonal spiral (DS) state and CF state for small n are due to the competition between the AF exchange interaction J and the fermion kinetic energy.

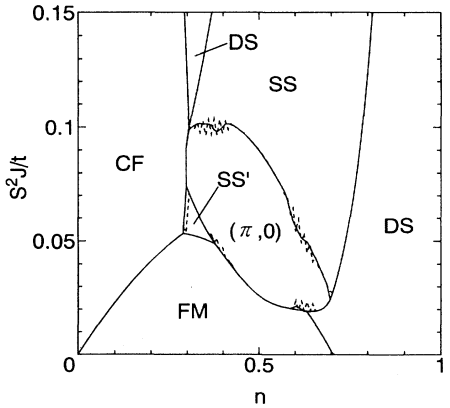

FIG. 1. The phase diagram in the ground state for $J_K=8t/S$. Solid lines and dotted lines are for system sizes 256×256 and 128×128. DS, SS, SS', and CF denote the phases of diagonal spiral state, stripe spiral state with $\mathbf{q}=(\pi,q_y)$ or (q_x,π), stripe spiral state with $\mathbf{q}=(q_x,0)$ or $(0,q_y)$, and canted ferromagnetic state, respectively. Here, $q_y\neq 0,\pi$ and $q_x\neq 0,\pi$.

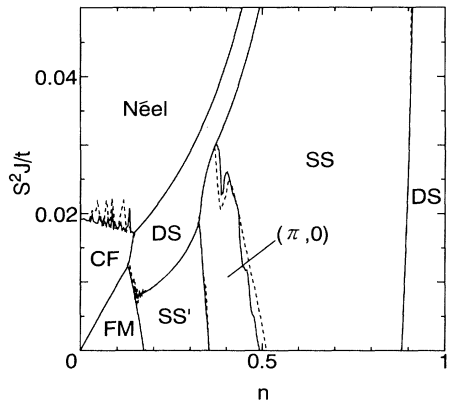

FIG. 2. The phase diagram in the ground state for $J_K=2t/S$. Solid lines and dotted lines are for system sizes 512×512 and 256×256. The notations of DS, SS, SS', and CF are the same as Fig. 1.

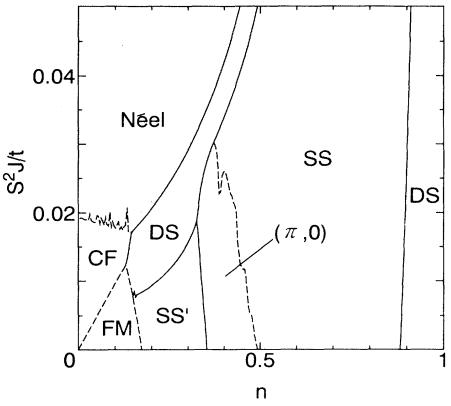

FIG. 3. Orders of transitions in the ground state. System size is 512×512. $J_K=2t/S$. Solid lines and broken lines denote first-order transition curves and second-order ones, respectively.

As increasing n, the fermion kinetic energy overcomes the AF exchange energy and the DS phase and the CF phases disappear. In the CF phase, the canting angle β_0 goes to zero as one approaches to $n=0$, and the state reduces to the Néel state.

On the other hand, for large n, Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions oscillating in space with the wave vector near (π,π) give rise to another DS phase. In particular, the spiral wave vector $\mathbf{q}$ continuously goes to (π,π) in the limit of $n\rightarrow1$. This is because the peak in the momentum dependence of the spin fluctuations of the fermions shifts to (π,π), and finally diverges at $n\rightarrow1$ as easily verified from the particle-hole symmetry.

Above the region of the ferromagnetic phase, we find regions of various stripe phases. We find a finite region of the state with $\mathbf{q}=(\pi,0)$, which is referred to as the $(\pi,0)$ state in this paper, and find a large area of the stripe spiral (SS) phase above that of the $(\pi,0)$ phase. In particular it is much larger than those of the DS phases and the CF phase in Fig. 2 for $J_K=2t/S$. This is interesting because J_K is of the order of t in copper oxide compounds, and the inelastic neutron-scattering experiments[15] show the incommensurate peaks at $\mathbf{q}=(\pm\pi,\pm\pi\pm\delta q_y)$ and $\mathbf{q}=(\pm\pi\pm\delta q_x,\pm\pi)$ in the wave-vector dependence of the spin fluctuations. The fermion concentrations for which the SS state appears are very different from those in the experiments. Nevertheless, this suggests at least that the SS state is possible also in a model in which spins on the Cu lattice sites are assumed to be localized.

Figure 3 is the phase diagram for $J_K=2t/S$ to show the order of phase transitions. The solid lines are first-order phase transition curves and the broken lines are second-order ones. It is found that the transition between the Néel state and the DS state for low densities is first order and that that between the CF state and the Néel state is second order. The canting angle of the CF state near the phase boundary of the Néel state continuously goes to zero as one approaches the Néel state.

To summarize, we have obtained the phase diagram of the spin-fermion model with classical localized spins. In spite of the simplicity of the treatment, our theory describes various mechanism of magnetic phenomena, such as double-exchange and RKKY interactions. As a result, our phase diagram consists of the Néel, ferromagnetic, canted ferromagnetic, diagonal spiral, stripe spiral, and $(\pi,0)$ phases. In particular, the large area of the stripe spiral phase is obtained for $J_K=2t/S$, which is consistent with the experimental results in the copper oxides.

For a close comparison to the copper oxides, we have to examine the spin-wave excitations to go beyond the classical-spin approximation and take into account the quantum fluctuations. In particular, the stability of the spiral states is the problem to be examined. However, our treatment is a good starting point because the classical-spin approximation can be regarded as taking the leading order of the spin-wave expansion.

On the other hand, our classical-spin model has much validity for compounds with large localized spins, such as $La_{1-x}Sr_xMnO_3$.[13,14] $La_{1-x}Sr_xMnO_3$ is three dimensional and has localized spins with $S=3/2\sim2$. Our calculation can be easily extended to the three-dimensional case. We expect that the phase diagram in the three-dimensional case would not be drastically different from the present result under the classical-spin approximation.

We have ignored the possibility of the phase separation in which fermions have spatially inhomogeneous distribution. However, this is justified, if we implicitly assume intersite or long-range Coulomb interactions between electrons and between electrons and atomic nuclei, which exist in the real materials and suppress such inhomogeneous states. When the phase separation occurs, the charge neutrality, including charges of dopants, is violated and such a state is apparently of high energy because of the Coulomb interactions. For example, in $La_{2-x}Sr_xCuO_4$, the charge neutrality must be kept in a large spatial scale, if one takes into account all charges of electrons and atomic nuclei of La, Sr, Cu, and O. Further, the Coulomb interactions between electrons also raise the total energy for such inhomogeneous states. To take into

account the correlation effects in the fermion system due to Coulomb interactions is another problem to be examined in the future.

We have not examined the nonplanar spiral spin states in this paper. We have found in the *t-J* model that nonplanar spiral states appear but the deviation from the planar spiral state is small.[9] Thus we expect that it is not poor approximation technique to ignore the nonplanar spiral states also in the present model. However, these problems should be explicitly examined in a future study.

ACKNOWLEDGMENTS

We are very grateful to Professor K. Nagai and Dr. H. Mori for useful discussions and encouragement. This work was partially supported by the Grant-in-Aid for Scientific Research from the Japanese Ministry of Education, Science and Culture. One of the authors (M.H.) acknowledges financial support from the Japan Society for the Promotion of Science.

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