Spin-flux phase in the Kondo lattice model with classical localized spins

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We provide numerical evidence that a spin-flux phase exists as a ground state of the Kondo lattice model with classical local spins on a square lattice. This state manifests itself as a double-Q magnetic order in the classical spins with spin density at both $(0,\pi)$ and $(\pi,0)$ and further exhibits fermionic spin currents around an elementary plaquette of the square lattice. We examine the spin-wave spectrum of this phase. We further discuss an extension to a face-centered-cubic (fcc) lattice where a spin-flux phase may also exist. On the fcc lattice the spin-flux phase manifests itself as a triple-Q magnetically ordered state and may exist in γ-Mn alloys.

The Kondo lattice model with classical local spins has emerged as one of the simplest models that can account for some of the physics of the manganites[1] and the cuprates.[2] For the manganites the ferromagnetic Kondo lattice model gives rise to the double exchange model which has been argued to be the relevant model to explain the physics in these materials.[3] For the cuprates the assumption of classical local spins is clearly unrealistic, however, the antiferromagnetic Kondo lattice model gives rise to many insights into high-T_c materials. For example, it has been used to understand the appearance of d-wave superconductivity[4–6] and it also gives rise to incommensurate magnetic[7,8] and stripe[7] structures that have been experimentally observed.[9,10] One aspect of this model that has recently gained interest is the appearance of a Berry phase in the fermion wave function that arises when the fermion spin is strongly pinned to the local classical spin orientation[11]. This Berry phase has been argued to give rise to a flux phase ground state on a square lattice in the manganites,[12] to an anomalous Hall effect in ferromagnets,[13] and to a quantized Hall conductance in Kagome lattices.[14] In this paper we examine the conditions under which this Berry phase gives rise to interesting ground-state structures. In particular, we give numerical evidence that a spin-flux phase appears as a ground-state structure of this model on a square lattice. This phase is analogous to but quite different from the flux phases that are usually discussed in the context of the cuprates.[15,16] The difference arises because the latter flux phases exhibit a finite current around each elementary plaquette of the square lattice, but in our case spin currents exist (for which the up and down electrons have opposite currents around an elementary plaquette). On the square lattice the phase discussed here has a spin flux of π through each elementary plaquette. In this regard, it is of interest to note that a π spin-flux phase has been argued to be central in explaining the normal-state properties of the cuprates by John and co-workers.[17]

In this paper we will first demonstrate numerically that a double-Q magnetic structure exists as a ground state of the Kondo lattice model. We then demonstrate that such a state is a spin-flux state with circulating spin currents and estimate the stability region of this phase. We also determine the spin-wave spectrum of the double-Q magnetic phase and demonstrate that a spin flux phase may exist for this model on a face-centered-cubic (fcc) lattice. The spin-flux phase on the fcc lattice manifests itself as a triple-Q magnetically ordered state and has a spin flux of $\pi/2$ through each elementary triangular plaquette that lies in the planes having Miller indices $(1,1,1)$ (and equivalent symmetry planes).

The model we study here is

$$H = -t \sum_{\langle \mathbf{ij} \rangle \alpha} (c^\dagger_{\mathbf{i}\alpha} c_{\mathbf{j}\alpha} + \text{H.c.}) - J \sum_{\mathbf{i}} \ \mathbf{s_i} \cdot \mathbf{S_i} + J' \sum_{\langle \mathbf{ij} \rangle} \ \mathbf{S_i} \cdot \mathbf{S_j},$$

(1)

where $c^\dagger_{\mathbf{i}\alpha}$ creates an electron at site $\mathbf{i} = (i_x, i_y)$ with spin projection α, $\mathbf{s_i} = \Sigma_{\alpha\beta} c^\dagger_{\mathbf{i}\alpha} \sigma_{\alpha\beta} c_{\mathbf{i}\beta}$ is the spin of the mobile electron, the Pauli matrices are denoted by σ, $\mathbf{S}_i$ is the localized spin at site $\mathbf{i}$, $\langle \mathbf{ij} \rangle$ denotes nearest-neighbor (NN) lattice sites, t is the NN-hopping amplitude for the electrons, J is a coupling between the spins of the mobile and localized degrees of freedom, and $J' > 0$ is a direct antiferromagnetic (AF) coupling between the localized classical spins. Throughout this paper the unit of energy will correspond to $t = 1$. The parameter $J > 0$ defines the ferromagnetic Kondo lattice model which has been argued to be relevant to the manganites; while $J < 0$ defines the antiferromagnetic Kondo lattice model which has been argued to be relevant to the cuprates. For the numerical studies a Monte Carlo technique was used. This involves no ''sign problems'' so that by this procedure temperatures as low as $T = 0.005$ at any density can be reached. The present study has been performed mostly on 6×6 lattices with periodic boundary conditions (PBC), but occasional runs were made also using open and antiperiodic BC as well as different lattice sizes (up to 12×12 lattices). The specific numerical technique used here involves a standard Metropolis algorithm for the classical spins and an exact diagonalization for the itinerant electrons. The details of the method are described in Ref. 18.

The spin-flux phase was identified numerically by studying the classical spin structure factor which is the Fourier
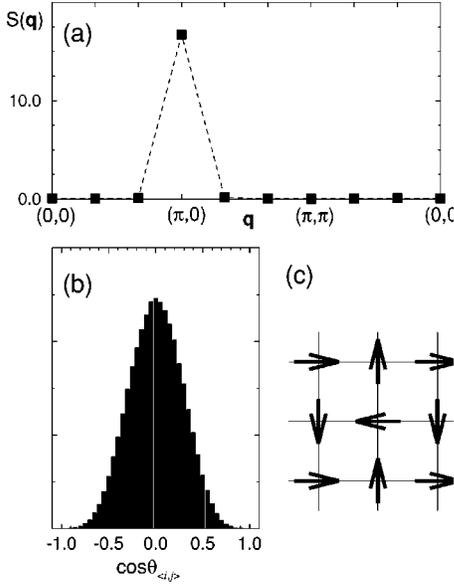
FIG. 1. (a) Structure factor $S(\mathbf{q})$, (b) histogram of snapshots for the nearest-neighbor spin dot product, (c) and resulting classical spin structure for $JS=2$, $J'S^2=0$, $T=1/200$, and $\langle n \rangle = 0.5$ on a 6 by 6 lattice with periodic boundary conditions.

transform of the static spin-spin correlation function $S(\mathbf{q})$ $=(1/N)\Sigma_{\mathbf{n},\mathbf{m}}e^{i\mathbf{q}\cdot(\mathbf{n}-\mathbf{m})}\langle \mathbf{S_n}\cdot\mathbf{S_m}\rangle$. In particular, it was found that for various JS and $J'S^2$ in the vicinity of electron density $\langle n \rangle = 0.5$ the structure factor was peaked at $\mathbf{Q}=(0,\pi)$ ($\mathbf{Q_y}$) and $\mathbf{Q}=(\pi,0)$ ($\mathbf{Q_x}$) (see Fig. 1).[19] To understand the possible ground states for a spin density with this wave vector it is useful to look at a Ginzburg Landau free energy. The order parameter is determined by the two vectors $\mathbf{M}_{0,\pi}$ and $\mathbf{M}_{\pi,0}$. The free energy can be simply constructed by noting that the relevant space-group representation transforms as a vector under spin rotations and as a scalar (that is, as an A_{1g}

representation) under the little co-group D_{2H} of the wave vector $\mathbf{Q}=(0,\pi)$. The most general dimensionless Ginzburg Landau free energy is

$$F = -(\mathbf{M}_{0,\pi}^2 + \mathbf{M}_{\pi,0}^2) + (\mathbf{M}_{0,\pi}^2 + \mathbf{M}_{\pi,0}^2)^2 + \beta\mathbf{M}_{0,\pi}^2\mathbf{M}_{\pi,0}^2$$
$$+ \beta_2(\mathbf{M}_{0,\pi}\cdot\mathbf{M}_{\pi,0})^2. \qquad (2)$$

The minimization of this energy leads to three possible ground states: (a) $(\mathbf{M}_{0,\pi},\mathbf{M}_{\pi,0})=(\mathbf{M},0)$, (b) $(\mathbf{M}_{0,\pi},\mathbf{M}_{\pi,0})$ $=(\mathbf{M}_1,\mathbf{M}_2)$ with $\mathbf{M}_1\cdot\mathbf{M}_2=0$, (c) $(\mathbf{M}_{0,\pi},\mathbf{M}_{\pi,0})=(\mathbf{M},\mathbf{M})$. The double-$Q$ phase (b) we will argue below is the spin-flux phase which in fact corresponds to a particular representation of flux phase proposed by Yamanaka et al.[12] [note that this phase does not lead to a peak in $S(\mathbf{q})$ at $(\pi/2,\pi/2)$ as suggested in Ref. 12]. The double-Q phase (c) corresponds to ordering only one half of the local moments and is therefore not a likely ground state for this model (note, however, that there exists numerical evidence for this phase in a periodic Anderson model on a square lattice[20]). To distinguish numerically which of these three phases corresponds to the phase found here the spin correlations were examined by evaluating $\mathbf{S_i}\cdot\mathbf{S_j}=S^2\cos\theta_{\langle ij\rangle}$ (the spin dot product of NN spins) for each pair of NN spins and plotting the value of $\cos\theta_{\langle ij\rangle}$ in a histogram. The results are shown in Fig. 1 for $JS=2$ and $J'S^2=0$. From this figure it is clear that NN spins are orthogonal which implies the double-Q order of phase (b) above.

To understand the electronic properties of this double-Q magnetic phase we fix the classical spins and find the fermion eigenstates [for the double-Q state this is reasonable because the spin structure factor is very strongly peaked at $(0,\pi)$ and $(\pi,0)$ with little weight at other $\mathbf{q}$ values as can be seen in Fig. 1]. The classical spin orientation is given by $\mathbf{S_i}$ $=(S/2)[(-1)^{i_x}+(-1)^{i_y},(-1)^{i_x}-(-1)^{i_y},0]$. Solving for the eigenstates of the resulting electronic Hamiltonian results in four bands with dispersions:

$$\epsilon_\mathbf{k}= \pm \sqrt{(JS)^2+4(\cos^2k_x+\cos^2k_y)\pm 2\sqrt{2(JS)^2(\cos^2k_x+\cos^2k_y)+16\cos^2k_x\cos^2k_y}}, \qquad (3)$$

where $(k_x,k_y)\in\{|k_x+k_y|\leqslant\pi\}\cap\{|k_x-k_y|\leqslant\pi\}$ are restricted to one-half the original Brillouin zone. The density of states (DOS) is linear in $|k|$ for $\langle n\rangle=0.5$ which is characteristic of the Dirac spectrum that appears for π-flux phases.[15,17] Also note that the dispersion relation is independent of the sign of J; consequently if this flux phase is the ground state for positive J then it must also be the ground state for negative J. In the limit $J=\infty$ the dispersion reduces to that found in Ref. 12. To identify this phase as a spin-flux state the spin current from site i to j was determined:

$$\mathbf{j}_{i,j}= it\sum_{\alpha,\beta}\langle c_{\alpha,i}^\dagger\sigma_{\alpha,\beta}c_{\beta,j}-c_{\alpha,j}^\dagger\sigma_{\alpha,\beta}c_{\beta,i}\rangle. \qquad (4)$$

It was found that only $[\mathbf{j}_{ij}]_z$ is nonzero and it is nonzero only for NN sites. The resulting spin currents circulate neighboring plaquettes in opposite directions. The charge current was

found to be zero. This spin current pattern implies a spin flux of π exists in each elementary plaquette. Note that in the limit $J=\infty$ this result is intuitively clear; in this limit the spin of the electron is tied to the local moment so that when the fermion travels around a plaquette the spin changes by 2π which implies that the wave function changes sign.

The phase diagram for $\langle n\rangle=0.5$ as a function of $1/(JS)$ and $J'S^2$ is shown in Fig. 2. The solid phase boundaries were found by comparing the energy of the flux phase to that of the canted magnetic and spin-density wave (SDW) phases (the energies of the helical SDW phases agree with those found in Ref. 8). At larger $J'S^2$ the flux phase is found to be unstable to a SDW phase characterized by $\mathbf{S_i}=\mathbf{S}\sqrt{2}$ $(-1)^{i_y}\cos(i_x\pi/2-\pi/4)$ (note that this is not a helical SDW state). This agrees with the structure found numerically.

It is of interest to determine the spin-wave spectrum arising from the spin-flux phase since this can be observed by
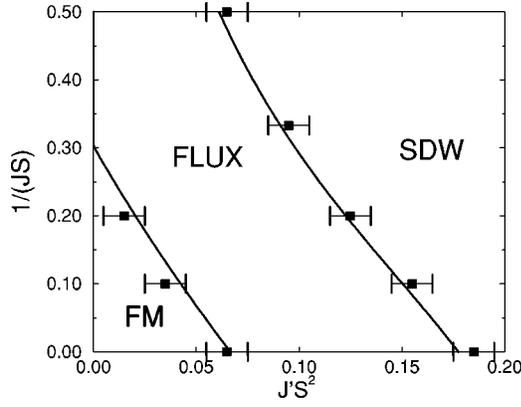
FIG. 2. Phase diagram for $\langle n \rangle = 0.5$. The filled squares represent the numerical results on a 6×6 lattice with $T = 1/200$ and with periodic boundary conditions.

inelastic neutron scattering. This can be done by using the spin-wave approximation that was introduced by Kubo and Ohata[21] and later used by Furukawa for the double exchange model.[22] The local spins are described by a local co-ordinate system in which each classical spin is aligned along the $\hat{z}$ direction and the spin-wave operators $S_i^+ \simeq \sqrt{2S} a_i$, $S_i^- \simeq \sqrt{2S} a_i^\dagger$, and $S_i^z = S - a_i^\dagger a_i$ are introduced. The spin-wave spectrum is found by keeping all $1/S$ corrections to the magnon self-energy. Here we consider the limit $J = \infty$. This results in the following effective boson Hamiltonian for the spin waves:

$$\sum_{\mathbf{k}} [\Pi(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + A(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{-\mathbf{k}} + \text{H.c.}] \quad (5)$$

with $\mathbf{k}$ summed over the whole Brillouin zone of the square lattice,

$$\Pi(\mathbf{k}) = \frac{1}{2SN} \sum_{\mathbf{q}} \left\{ E_{\mathbf{q}} - \cos(\theta_{\mathbf{q}} - \theta_{\mathbf{k}+\mathbf{q}}) E_{\mathbf{k}+\mathbf{q}} - \frac{E_{\mathbf{k}+\mathbf{q}}^2}{E_{\mathbf{q}} + E_{\mathbf{k}+\mathbf{q}}} \right.$$
$$\left. \times [1 - \cos(5\theta_{\mathbf{k}+\mathbf{q}} - \theta_{\mathbf{q}})] \right\} + J'S(\cos k_x + \cos k_y), \quad (6)$$

$$A(\mathbf{k}) = \frac{1}{2SN} \sum_{\mathbf{q}} \frac{E_{\mathbf{k}+\mathbf{q}} E_{\mathbf{q}}}{E_{\mathbf{q}} + E_{\mathbf{k}+\mathbf{q}}} [\cos(2\theta_{\mathbf{q}} + 2\theta_{\mathbf{k}+\mathbf{q}}) - \cos(\theta_{\mathbf{q}} - \theta_{\mathbf{k}+\mathbf{q}})] + J'S(\cos k_x + \cos k_y), \quad (7)$$

$\cos\theta_{\mathbf{k}} = [\cos k_x + \cos k_y]/E_{\mathbf{k}}$, $\sin\theta_{\mathbf{k}} = [\cos k_x - \cos k_y]/E_{\mathbf{k}}$, and $E_{\mathbf{k}} = \sqrt{2}\sqrt{\cos^2 k_x + \cos^2 k_y}$. The spin-wave dispersion is given by $\omega_{\mathbf{k}}^2 = \sqrt{\Pi(\mathbf{k})^2 - |A(\mathbf{k})|^2}$. The eigenstate of this mode is given by $\delta S_{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \{ e^{i\mathbf{Q}_x\cdot\mathbf{r}} [\Pi(\mathbf{q}) + A(\mathbf{q})][(\hat{x} + \hat{y})/2] + i\omega_{\mathbf{q}}\hat{z} + e^{i\mathbf{Q}_y\cdot\mathbf{r}}[\Pi(\mathbf{q}) + A(\mathbf{q})][(\hat{y} - \hat{x})/2] \}$ (recall the ordered moment is $\mathbf{S}_0(\mathbf{r}) = e^{i\mathbf{Q}_x\cdot\mathbf{r}}[(\hat{x} + \hat{y})/2] + e^{i\mathbf{Q}_y\cdot\mathbf{r}}[(\hat{x} - \hat{y})/2]$). The resulting spin-wave spectrum (see Fig. 3) agrees with the general form required by phenomenological arguments (found by using the method of Zhu and Walker[23]).

Given that the spin-flux phase was found to be stable on a square lattice it is natural to ask whether such states can be realized on other lattice structures. We argue that a spin-flux
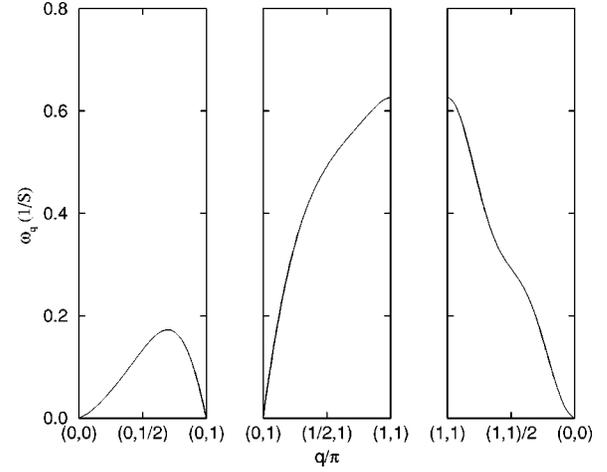

FIG. 3. Magnon dispersion relation for the double-Q magnetic phase ($J'S^2 = 0.1$).

phase is likely to be stable on a fcc lattice. For an fcc lattice two degenerate ground states of the NN classical Heisenberg model are $\mathbf{S}_{3Q}(\mathbf{R}) = [(-1)^{l_1+l_2}, (-1)^{l_2+l_3}, (-1)^{l_2+l_3}]/\sqrt{3}$ and $\mathbf{S}_{1Q}(\mathbf{R}) = [(-1)^{l_1+l_2}, 0, 0]$ where the fcc lattice is spanned by $\mathbf{R} = [l_1 a(\hat{x} + \hat{y})/2, l_2 a(\hat{x} + \hat{z})/2, l_3 a(\hat{y} + \hat{z})/2]$ (note that there exists a continuous degeneracy in the ground state, but in the presence of the Kondo coupling only two states are relevant). In the limit $J = \infty$ the structure $\mathbf{S}_{3Q}$ gives rise to a spin-flux phase with the spectrum

$$\epsilon_{\mathbf{k}} = \pm \frac{4}{\sqrt{3}} \sqrt{\cos^2\frac{k_x}{2}\cos^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\cos^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\cos^2\frac{k_x}{2}}, \quad (8)$$

where the momenta are restricted to the region of the Brillouin zone where $-2\pi < k_z < 0$. Note that for $\langle n \rangle = 0.5$ the DOS is again linear in energy. For the structure $\mathbf{S}_{1Q}$ the dispersion is $\epsilon_k = -4t \cos(k_x/2)\cos(k_y/2)$. Assuming that one of these ground states is stable (that is taking J' to be sufficiently large) then it is found that at $\langle n \rangle = 1$ the $\mathbf{S}_{1Q}$ state is stable while at $\langle n \rangle = 0.5$ the $\mathbf{S}_{3Q}$ state is stable. There is a transition between these two states at $\langle n \rangle = 0.7$. As in the case of the square lattice the $\mathbf{S}_{3Q}$ phase has no net current flowing about any closed loops on the lattice but it has spin currents flowing around the elemental triangular plaquettes that exist in planes with Miller indices $(1,1,1)$ (and equivalent symmetry planes). The spin currents that flow correspond to a spin flux of $\pi/2$ per triangular elemental plaquette (not π per plaquette as was the case in the square lattice). It is intriguing to note that Hasegawa et al. have pointed out that for a triangular lattice the optimal flux per plaquette in a $U(1)$ flux phase is $\pi/2$ at $\langle n \rangle = 0.5$.[16] Both the $\mathbf{S}_{1Q}$ and the $\mathbf{S}_{3Q}$ states have been observed in γ-Mn alloys produced by doping with Fe, Ni, or Cu,[24,25] and it would be of interest to see if an electronic pseudogap or spin currents can be detected in the $\mathbf{S}_{3Q}$ phase of these materials.

In conclusion, we have given numerical evidence that a spin-flux phase exists as a ground state of the Kondo lattice model with classical localized spins on a square lattice. This phase gives rise to a spin flux of π for electrons circulating

an elementary plaquette of the square lattice and manifests itself as a double-Q magnetic order in the classical spins. We have also proposed that a spin-flux phase may be stable on a fcc lattice. This phase manifests itself as a triple-Q magnetic order and gives rise to a spin flux of $\pi/2$ for electrons circulating the elementary triangular plaquettes that lie in the planes with Miller indices $(1,1,1)$ (and equivalent symmetry planes).

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