Chiral helimagnetic state in a Kondo lattice model with the Dzyaloshinskii–Moriya interaction

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Abstract
Monoaxial chiral magnets can form a noncollinear twisted spin structure called the chiral helimagnetic state. We study magnetic properties of such a chiral helimagnetic state, with emphasis on the effect of itinerant electrons. Modeling a monoaxial chiral helimagnet by a one-dimensional Kondo lattice model with the Dzyaloshinskii–Moriya interaction, we perform a variational calculation to elucidate the stable spin configuration in the ground state. We obtain a chiral helimagnetic state as a candidate for the ground state, whose helical pitch is modulated by the model parameters: the Kondo coupling, the Dzyaloshinskii–Moriya interaction, and electron filling.

Keywords: chiral magnet, Kondo lattice model, Dzyaloshinskii–Moriya interaction, variational calculation

1. Introduction

Chirality in the lattice structure plays an important role in magnetism through the spin–orbit coupling which couples the orbital motion of electrons and the spin degree of freedom. It often leads to noncollinear and noncoplanar spin textures, such as a chiral helimagnetic (CHM) state \cite{1, 2, 3} and a skyrmion crystal \cite{4, 5, 6}. Such peculiar spin textures have attracted attention as they may result in unusual magnetoelectric phenomena, e.g., the topological Hall effect \cite{7, 8, 9} and the spin Hall effect \cite{10}.

An archetypal example of the CHM state is found in CrNb$_3$S$_6$, which is a monoaxial chiral magnet with space group of P6$_3$22. At low temperatures, the compound exhibits a CHM order at zero magnetic field, while it turns into a chiral soliton lattice (CSL) in the magnetic field applied perpendicular to the chiral axis \cite{11, 12}. The CHM and CSL states were observed by using the Lorentz microscopy with a transmission electron microscope and the small-angle electron diffraction \cite{13}. Theoretically, since the pioneering work by Dzyaloshinskii \cite{1, 14}, the CHM and CSL states have been studied for decades, whereas the most of them were limited to localized spin systems by omitting the degree of freedom for itinerant electrons \cite{15, 16, 17, 18}. Recently, the authors studied this problem by explicitly taking into account the coupling to itinerant electrons \cite{19}. Monte Carlo simulations for an extended Kondo lattice model with the Dzyaloshinskii–Moriya (DM) interaction \cite{20, 21} successfully explain a correlation between the twist of CSL and the electrical conduction.

In this paper, we report our theoretical study for the ground state of the extended Kondo lattice model whose finite-temperature properties were studied by the Monte Carlo simulations. Focusing on the zero-field state, we obtain the stable magnetic configuration in the ground state by a variational calculation. We find that the model exhibits a CHM state whose helical pitch depends on the model parameters: the Kondo coupling, the DM interaction, and electron filling. Our results elucidate how the CHM state is stabilized by the competition between the DM interaction and an effective exchange interaction mediated by itinerant electrons.

The organization of this paper is as follows. In Section \ref{sec:ModelMethod} we introduce a ferromagnetic Kondo lattice model with the DM interaction and the method of variational calculations. The results for the optimized magnetic structures are shown in Section \ref{sec:Results}. Section \ref{sec:Discussion} is devoted to the summary.

2. Model and method

Following the previous study \cite{19}, we consider a ferromagnetic Kondo lattice model with the DM interaction between the localized spins in one dimension. The
Hamiltonian is given by

\[
H = -t \sum_{l,\nu} (c_{l\nu}^\dagger c_{l+1\nu} + \text{h.c.}) - \mu \sum_{l,\nu} c_{l\nu}^\dagger c_{l\nu} \\
- J \sum_{l,\nu,\rho} c_{l\nu}^\dagger \sigma_{\nu\rho} c_{l\rho} \cdot S_l - D \cdot \sum_l S_l \times S_{l+1},
\]

(1)

where \(c_{l\nu}(c_{l\nu}^\dagger)\) is an annihilation (creation) operator for a \(\nu\)-spin electron at site \(l\) on the one-dimensional chain (\(\nu = \uparrow\) or \(\downarrow\)), \(\mu\) is the chemical potential, and \(S_l = (S_l^x, S_l^y, S_l^z)\) is a three-component vector with normalized length \(|S_l| = 1\). We assume the periodic boundary condition. The first term describes the kinetic energy of itinerant electrons; \(t\) is a transfer integral between the nearest-neighbor sites. The third term is for the onsite coupling between the itinerant electrons and localized moments; \(J\) is a positive coupling constant and \(\sigma = (\sigma^x, \sigma^y, \sigma^z)\) are the Pauli matrices. The last term represents the DM interaction with the DM vector \(\mathbf{D} = D\hat{z}\), where \(D > 0\) and \(\hat{z}\) is a unit vector along the chain direction. In this study, we focus on the case in the absence of a magnetic field.

We study the ground state of the model in equation (1) by a variational calculation. As the variational ground state, we assume a helical spin configuration represented by

\[
S_l = (\cos Ql, \sin Ql, 0),
\]

(2)

where \(Q\) is the wave number related with the helical pitch \(L\) as \(L = 2\pi/Q\) (we set the lattice constant as the length unit). For the spin configuration, we can calculate the energy dispersion of itinerant electrons as

\[
\varepsilon(k) = -2t \cos k \cos \frac{Q}{2} - \mu \\
\pm \sqrt{2^2(1 - \cos 2k)(1 - \cos Q) + J^2}.
\]

(3)

Then, we can compute the total energy of the system by

\[
E = \sum_{-k_F \leq k \leq k_F} \varepsilon(k) - DN \sin Q,
\]

(4)

where \(k_F\) is the Fermi wave number [\(\varepsilon(k_F) = \mu\)] and \(N\) is the number of sites. In the variational calculations, we optimize \(E\) by varying \(Q\) while tuning the chemical potential \(\mu\) to set the electron filling \(n\) at a particular value. The electron filling \(n\) is defined by the average number of electrons per site: \(n = \frac{1}{N} \sum_{-k_F \leq k \leq k_F} 1\), which varies from 0 to 2. The optimal value of \(Q\), which we denote as \(Q^*\), defines the pitch for the most stable helical spin configuration. We set the energy unit \(t = 1\) and take \(N = 10^4\) in the following calculations.

3. Result

Figure 1 shows the result for the optimal wave number \(Q^*\) as a function of \(J\) and \(D\) at quarter filling \(n = 0.5\). When \(D = 0\), an infinitesimal \(J\) induces a helimagnetic order (without chirality) with the optimal wave number \(Q^* = \pi/2\). This is due to the Ruderman–Kittel–Kasuya–Yosida interaction \([22, 23, 24]\) dictated by the twice of the Fermi wave number \(2k_F = \pi/2\) at quarter filling \(n = 0.5\).

While increasing \(J\) at \(D = 0\), \(Q^*\) becomes smaller (namely, the helical pitch becomes longer), and \(Q^*\) vanishes for \(J \gtrsim 1.6\), as shown in Fig. 1. This indicates that the lowest-energy state is given by a single ferromagnetic order without any twist for \(J \gtrsim 1.6\) at \(D = 0\). The ferromagnetic state is stabilized by the effective ferromagnetic interaction mediated by the kinetic motion of itinerant electrons, called the double-exchange interaction \([25, 26]\).

When \(D\) is turned on, \(Q^*\) increases as \(D\) increases (except for \(J = 0\)). As shown in Fig. 1, however, the increase of \(Q^*\) becomes slower for larger \(J\). This is because the effective magnetic interaction mediated by itinerant electrons becomes stronger for a larger \(J\). In the limit of \(D \to \infty\), the system prefers the helical order with \(\pi/2\) rotation of spins between neighboring sites for any value of \(J\), and hence, \(Q^*\) converges to \(\pi/2\).

We also investigate the \(n\) dependence of the optimal wave number \(Q^*\). Figure 2 displays the values of \(Q^*/2\pi\) as functions of \(D\) at several electron fillings \(n\) for \(J = 2\). At a low filling, for instance, at \(n = 0.1\), \(Q^*\) is zero at \(D = 0\) (ferromagnetic state) and grows gradually as \(D\) increases (CHM state). The growth rate is suppressed as \(n\) increases because the effective ferromagnetic interac-
It is expected in this system, as mentioned in Sec. 1. It would be interesting to extend our variational study for investigating the optimal magnetic state while changing the magnetic field. In particular, it is an intriguing issue to clarify the role of itinerant electrons in the CSL state, by comparing with the previous results for the models with localized spins only.

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