

Partially disordered states of the three-dimensional ANNNI model

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Abstract

We analyze the three-dimensional axial next-nearest-neighbor Ising (ANNNI) model composed of two kinds of alternately stacked ferromagnetic layers with different intralayer interactions by using Monte Carlo (MC) simulation. The detailed analyses of the magnetization and the spin correlations perpendicular to the stacked direction, assure and clarify the existence and the nature of the paramagnetic layers in some modulated phases with wave numbers, 1/4, 1/8, 3/16. This is the first MC confirmation of the partially disordered states which have been predicted by previous molecular field calculation and/or observed in materials such as CsCoCl₃, CuFeO₂ and CeSb.

Key words: ANNNI model; molecular-field calculation; Monte Carlo simulation; partially disordered states

The three-dimensional (3D) axial next-nearest-neighbor Ising (ANNNI) model [1,2] is a particularly simple model exhibiting spacially modulated phases which can be either commensurate or incommensurate with the underlying lattice. Theoretical studies [1,2] have revealed successive phase transitions, called “devil’s staircase”, similar to the behavior of rare-earth metals and their compounds.

The partially disordered state (PDS) is the ordered state including paramagnetic spins and experimentally observed in CsCoCl₃ [3], CeSb [4] and so on. By employing the antiferromagnetic triangular lattice with geometric frustration, Mekata and Adachi explained the phase transitions in CsCoCl₃ [3]. On the other hand, the 3D ANNNI model with competing interactions was proposed in order to understand the phase transitions and the ordered states in CeSb. In this model, however, the PDS suggested by the molecular-field approximation [5] was denied by the calculation based on the transfer matrix method [6] and Monte Carlo (MC) simulation [7]. Although ANNNI model could reproduce the successive phase transitions and

the ordered states in CeSb qualitatively, PDS could not be reproduced. Therefore, it is important to propose extended model which stabilizes the PDS.

In previous study [8], the extended 3D ANNNI model described by the following Hamiltonian was proposed;

$$\mathcal{H} = -J_0 \sum_{\langle i,j \rangle} S_i S_j - J'_0 \sum_{\langle i,j \rangle} \mu_i \mu_j - J_1 \sum_{\langle i,j \rangle} S_i \mu_j - J_2 \sum_{\langle i,j \rangle} S_i S_j - J'_2 \sum_{\langle i,j \rangle} \mu_i \mu_j. \quad (1)$$

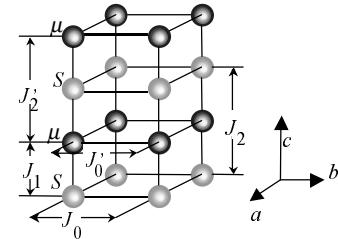


Fig. 1. The extended 3D ANNNI model.

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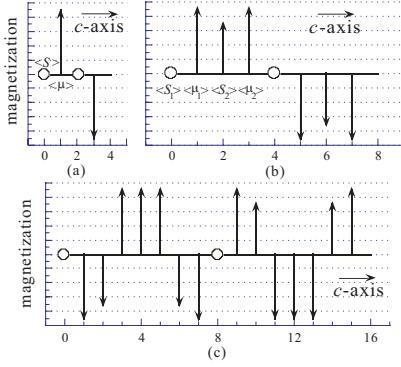


Fig. 2. Spin configurations along the c -axis in PDS with (a) $k = 1/4$, (b) $k = 1/8$ and (c) $k = 3/16$ predicted by MFA.

This model is composed of two kinds of alternately stacked ferromagnetic layers. These layers consist of spins $S_i (= \pm 1/2)$ or $\mu_i (= \pm 1/2)$, and are termed S -layer or μ -layer. J_0 and J'_0 are the nearest-neighbor ($n.n.$) intralayer ferromagnetic interactions in S -layer and μ -layer, respectively. $J_1 > 0$, $J_2 < 0$, and $J'_2 < 0$ are the $n.n.$ interlayer interaction, the next-nearest-neighbor ($n.n.n.$) interlayer interaction between S -layers and the $n.n.n.$ interlayer interaction between μ -layers, respectively (Fig.1). The summation is taken over the $n.n.$ and the $n.n.n.$ pairs of sites.

In our previous paper, we applied the molecular-field approximation (MFA) to the extended ANNNI model and showed that PDS with wave numbers, $k = 1/4, 1/8$ and $3/16$ appeared in the magnetic phase diagram [8]. The spin configurations along the c -axis in PDS with $k = 1/4, 1/8$ and $3/16$ are shown in Fig.2, where arrow and circle indicate the thermal average of magnetization in each layer and a paramagnetic layer, respectively. However, the results obtained by MFA are not conclusive, as we have seen in the case of the ordinary ANNNI model[5–7]. In this paper, therefore, by means of MC method, we confirm the existence of the PDS with $k = 1/4, 1/8$ and $3/16$ predicted by MFA.

For $\kappa (\equiv J_2/J_1 = J'_2/J_1) = -0.9 \sim -0.4$, under the condition of $J_0/J_1 = 0.5$ and $J'_0/J_1 = 1.0$, the MC calculations were performed on $L \times L \times L_z$ ($L = 20 \sim 90, L_z = 40, 48$) simple cubic lattice with periodic boundary conditions. Spin updating followed a Metropolis dynamics. Thermal averages were calculated using 2×10^4 Monte Carlo steps per spin (MCS) after equilibrating with initial 10^5 MCS.

For $k_B T/J_1 = 0.675$ and $\kappa = -0.4$, where $k = 1/8$ PDS is expected, the least-square fitting plots of the size dependence of layer magnetizations, $\langle S_1 \rangle, \langle S_2 \rangle, \langle \mu_1 \rangle$ and $\langle \mu_2 \rangle$ are shown in Fig.3, where $\langle \mu_2 \rangle$ is omitted due to no differences between $\langle \mu_1 \rangle$ and $\langle \mu_2 \rangle$. Although $\langle S_1 \rangle$ has a small finite value in each lattice size owing to the finite-size effect, the least-square fitting plots of the size dependence of $\langle S_1 \rangle$

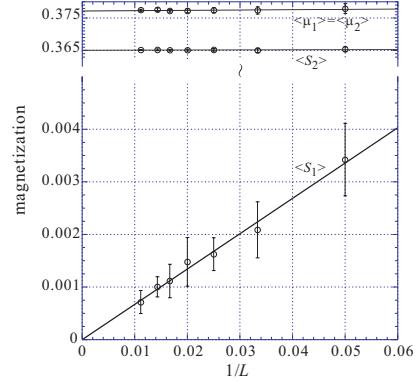


Fig. 3. For $k_B T/J_1 = 0.675$ and $\kappa = -0.4$, the least-square fitting plots of the size dependence of layer magnetizations.

shows $\langle S_1 \rangle = (0.15 \pm 1.7) \times 10^{-4}$ in the thermodynamical limit, that is, the paramagnetic state. On the other hand, the least-square fitting plots of the size dependence of $\langle S_2 \rangle$ and $\langle \mu_1 \rangle$ show that these have finite values in the thermodynamical limit. Fig.3, therefore, shows that the state for $k_B T/J_1 = 0.675$ and $\kappa = -0.4$ is the $k = 1/8$ PDS. A similar analysis of MC data for other combinations of $k_B T/J_1$ and κ also shows the existence of the PDS with $k = 1/4$ and $3/16$.

Intralayer spin correlations in S -layer and μ -layer are calculated by MC method. For $k_B T/J_1 = 0.675, \kappa = -0.4$ and $L_z = 48$, the correlation in S_1 -layer decays to 0 for only five sites distance. On the other hand, those in other layers decay over a few sites but remain finite. The intralayer spin correlations also show that the state for $k_B T/J_1 = 0.675$ and $\kappa = -0.4$ is the PDS.

We analyzed the extended ANNNI model by MC simulation. The detailed analyses of the magnetization and the spin correlations assure and clarify the existence of the PDS. These PDS are incomprehensible without the alternation of intralayer interactions as well as the competition of J_1 with J_2 and J'_2 . The investigation of the nature of phase boundaries between PDS and adjacent phases is now in progress.

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