Exchange striction model for the spin configuration in the antiferromagnetic YMn_2 with the cubic Laves phase structure

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Abstract

By making use of the Luttinger-Tisza method for the classical spin Heisenberg model, we examine how the exchange striction affects the highly frustrated pyrochlore-type spin system in YMn_2 with the cubic Laves phase (C15) structure. The distance dependence of the exchange parameter between the nearest neighboring spin pair is taken into account. The complicated spin configuration observed in YMn_2 is deduced through energy change due to the exchange striction.

Key words: frustrated antiferromagnetism; YMn_2; exchange striction; pyrochlore-type spin system

In the intermetallic compound of YMn_2 with the cubic Laves phase (C15) structure, the Mn atom has a large magnetic moment and orders in a complicated spin configuration [1], which is referred to as NSK configuration hereafter. The Mn atoms compose a highly frustrated pyrochlore-type spin system. The spin configuration has been investigated on the basis of the classical spin Heisenberg model before [2,3]. In the present paper, we show that the two collinear configurations of the NSK and of the layered one are possible for the nearest neighbor interaction model if exchange striction is taken into account.

The energy for the spin system with the nearest neighbor interaction is written as

$$E_{\rm ex} = -\sum_{\text{n.n. pair}} J\,\boldsymbol{S}_{n\nu}\cdot\boldsymbol{S}_{m\mu}, \qquad (1)$$

where $\boldsymbol{S}_{n\nu}$ is the spin vector on the ν-th Mn atom in the n-th unit cell and J is assumed to be negative. $E_{\rm ex}$ is minimized under the constraint $|\boldsymbol{S}_{n\nu}| = S$ to determine the spin configuration. We restrict our consideration to the simple case where the spin is a classical one and the configuration is described by a single modulation wave vectors as $\boldsymbol{S}_{n\nu} = \boldsymbol{S}_\nu(\boldsymbol{q})\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_{n\nu}) + \text{c.c.}$, where $\boldsymbol{R}_{n\nu} = \boldsymbol{R}_n + \boldsymbol{r}_\nu$ represents the position of the ν-th Mn atom, $\nu = 1 \sim 4$, in the n-th unit cell and $\boldsymbol{R}_n = (n+l, l+m, m+n)(a/2)$ for the fcc space lattice with lattice constant a. By the condition that $\boldsymbol{S}_{n\nu}$ is real, we can write $\boldsymbol{S}_\nu(\boldsymbol{q}) = S\,u_\nu(\boldsymbol{q})\,[\boldsymbol{i}(\boldsymbol{q}) - \mathrm{i}\boldsymbol{j}(\boldsymbol{q})]/2$, where $\boldsymbol{i}(\boldsymbol{q})$ and $\boldsymbol{j}(\boldsymbol{q})$ are a set of orthonormal real vectors and $u_\nu(\boldsymbol{q})$ is a phase factor. The energy and constraint are represented as

$$E_{\rm ex} = -(NS^2/2)\sum_{\nu,\mu} J_{\nu\mu}(\boldsymbol{q})\,u_\nu(\boldsymbol{q})^* u_\mu(\boldsymbol{q}) \qquad (2)$$

and $u_\nu(\boldsymbol{q})u_\nu(\boldsymbol{q})^* = 1$, where $J_{\nu\mu}(\boldsymbol{q}) = \sum J\exp[\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_{m\mu} - \boldsymbol{R}_{n\nu})]$. Following the prescription by Luttinger and Tisza [4], our problem is reduced to an eigenvalue problem,

$$\sum_\mu J_{\nu\mu}(\boldsymbol{q})u_\mu(\boldsymbol{q}) = \Lambda u_\nu(\boldsymbol{q}), \qquad (3)$$

with the Lagrange's undetermined multiplier Λ. The $\boldsymbol{S}_{n\nu}$ corresponding to the *eigen-vector* $\boldsymbol{u} = (u_1, u_2, u_3, u_4)$ is given by

$$S[\cos(\boldsymbol{q}\cdot\boldsymbol{R}_n + \psi_\nu)\,\boldsymbol{i} + \sin(\boldsymbol{q}\cdot\boldsymbol{R}_n + \psi_\nu)\,\boldsymbol{j}], \qquad (4)$$

where $\psi_\nu = \boldsymbol{q}\cdot\boldsymbol{r}_\nu + \theta_\nu$ and θ_ν is the phase angle of $u_\nu(\boldsymbol{q})$. For the modulation vectors $\boldsymbol{q}$ in the directions

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of Δ and Σ axes in the Brillouin zone with arbitrary length $|\boldsymbol{q}|$, all the energies are shown to be degenarate and to give the lowest energy [2], in other words, the ground state is highly frustrated.

In the direction of Δ axis, the spins with the modulation vector $\boldsymbol{q} = (0, 0, \zeta)(4/a)$ are given as $\boldsymbol{S}_{n1} = S\{\cos[2(m+n)\zeta]\boldsymbol{i} + \sin[2(m+n)\zeta]\boldsymbol{j}\} = -\boldsymbol{S}_{n2}$ and $\boldsymbol{S}_{n3} = S\{\cos[2(m+n)\zeta+\phi]\boldsymbol{i} + \sin[2(m+n)\zeta+\phi]\boldsymbol{j}\} = -\boldsymbol{S}_{n4}$ with an arbitrary ϕ, which give the NSK configuration if $\zeta = \pi/2$, i.e., $\boldsymbol{q}$ at the X point on the zone surface as well as $\phi = 0$ or π.

Now, we take into account the exchange striction effect. By putting the change in distance between the nearest neghboring pair as $\delta|\boldsymbol{r}_{m\mu,n\nu}| = r_0\rho_{m\mu,n\nu}$, we have

$$J(|\boldsymbol{r}_{m\mu,n,\nu}|)/J_0 = 1 + \gamma\rho_{m\mu,n\nu}, \tag{5}$$

where $\gamma = \mathrm{d}\ln|J|/\mathrm{d}\ln r$. Then,

$$\delta E_{\mathrm{ex}} = -(J_0/2)\sum \gamma\rho_{n\nu,m\mu}\boldsymbol{S}_{n\nu}\cdot\boldsymbol{S}_{m\mu}. \tag{6}$$

We approximate the elastic energy by a pair model as

$$\delta E_{\mathrm{el}} = (k/2)\sum_{\text{n.n. pair}}(\rho_{n\nu,m\mu})^2, \tag{7}$$

where k is force constant. By minimizing $\delta E = \delta E_{\mathrm{ex}} + \delta E_{\mathrm{el}}$ with respect to $\rho_{n\nu,m\mu}$, we have $\rho_{m\mu,n\nu} = (J_0\gamma/k)\boldsymbol{S}_{n\nu}\cdot\boldsymbol{S}_{m\mu}$. Thus, the change in energy due to the exchange striction is given by

$$\delta E = -(J_0^2/4)\gamma^2/k\sum(\boldsymbol{S}_{n\nu}\cdot\boldsymbol{S}_{m\mu})^2 \tag{8}$$

$$= -(J_0^2/8)N\gamma^2S^4/k\sum u_\nu^2u_\mu^{*2}\cos 2\boldsymbol{q}\cdot\boldsymbol{r}_{\nu\mu} + \text{const.}$$

For $\boldsymbol{q} = (0, 0, \zeta)(4/a)$ along Δ axis, we have a doubly degenerate solution and the eigen-vectors are given [2] by $\boldsymbol{u}_\Delta = (1, -1, \pm\mathrm{e}^{\mathrm{i}\theta}, \mp\mathrm{e}^{\mathrm{i}\theta})$. The energy change is estimated by the first order perturbation [2,3] as

$$\delta E = -(J_0^2NS^4\gamma^2/2k)(1 + 2\cos 2\zeta\cos 2\theta). \tag{9}$$

The minimum value is obtained for the case of

$$\theta = \pi/2 \quad \text{and} \quad \zeta = \pi/2, \tag{10}$$

i.e., at X point, which gives the NSK configuration, and for the case of

$$\theta = 0, \pi \quad \text{and} \quad \zeta = 0, \tag{11}$$

i.e., at Γ point, which gives a layered antiferromagnetic configuration. The degeneracy of the solutions at X and Γ points can be removed by second and/or third neighbor interactions [3]. For the solution for $\boldsymbol{q}$ in direction of the Σ axis, we have a doubly degenerate solution and eigen-vectors are given [2] as $\boldsymbol{u}_\Sigma = (1, -\mathrm{e}^{\pm\mathrm{i}\zeta}, -\mathrm{e}^{\mp\mathrm{i}\zeta}, 1)$, where ζ varies from 0 at Γ point to $3\pi/8$ at K point in the Brillouin zone. Then, we have $\delta E = -(J_0NS^4\gamma^2/2k)(1 + 2\cos 4\zeta)$, which gives the minimum value at $\zeta = 0$, i.e., at Γ point.

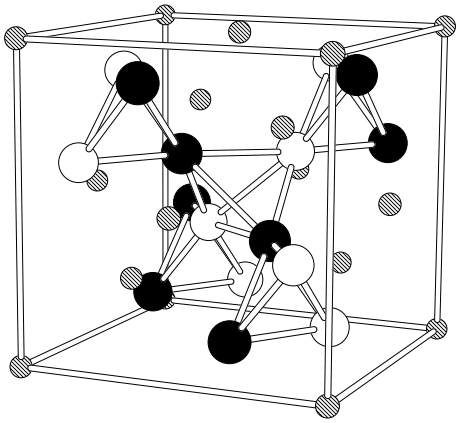

Fig. 1. A model of the distorted C15 lattice for the antiferromagnetic YMn_2. The closed and open circles represent the Mn atoms with the up and down moment. The small gray circles represent the nonmagnetic Y atoms

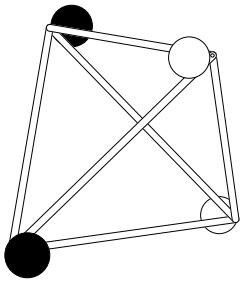

Fig. 2. Displacement of Mn atoms in a tetrahedron.

Usually, it is expected that the distance between parallel spin pair is greater the that between anti-parallel one by the Pauli exclusion principle. And a tetragonal distortion of $c/a < 1$ is actually observed in [5]. Then, to make these conditions compatible, we propose a distorted C15 lattice as shown in Fig.1. The displacement of each Mn atom in a tetrahedron is shown in Fig.2.

In conclusion, the NSK configuration for the antiferromagnetic YMn_2 is deduced on the basis of the classical spin Heisenberg model by taking into account the exchange striction effect and the distorted C15 lattice is proposed in the present paper.

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