with (1, 0, 0). The detail of our phase diagram is rather different from that proposed by Yoshimori.[2] We use a numerical calculation approach in finding the distribution of the magnetic Bragg peaks in the fixed reciprocal lattice planes such as (h, k, l) with one index fixed. To this end we calculate the equi-energy contour plot of the negative sign of the Fourier transform of the spin Hamiltonian, $J(h, k, l)$. The magnetic Bragg peaks are located inside the maximum equi-energy contour. The selection rule for the location of the magnetic Bragg peaks is the same as that derived by Yoshimori.[2] This numerical method has an advantage in visualizing the location of the magnetic Bragg peaks in the reciprocal lattice space. The nature of the phase transitions on the phase boundaries will be discussed.

II. BACKGROUND: GENERAL THEORY FOR THE ORDERED SPIN STRUCTURE

We follow the theory presented by Nagamiya.[9] We consider a lattice of magnetic atoms such as β-MnO_2. The unit cell can be chosen so that it contains one magnetic atom. On each magnetic atom, we assume a *classical spin*. Between the spin $\mathbf{S}_i$ at the position $\mathbf{R}_i$ and $\mathbf{S}_j$ at $\mathbf{R}_j$, there is an Heisenberg-type exchange interaction. The Heisenberg spin Hamiltonian is expressed by

$$H = -2\sum_{i,j} J(\mathbf{R}_{ij})\mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where

$$J(-\mathbf{R}_{ij}) = J(\mathbf{R}_{ij}),$$

and

$$\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j.$$

The exchange interaction $J(\mathbf{R}_{ij})$ is not restricted to the nearest neighbors. We now use the Fourier transformations of the exchange interaction and spin;

$$J(\mathbf{q}) = \sum_{j(\neq i)} J(\mathbf{R}_{ij}) \exp(-i\mathbf{q} \cdot \mathbf{R}_{ij}), \tag{2}$$

$$\mathbf{S}_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \mathbf{S}_{\mathbf{q}} \exp(iq \cdot \mathbf{R}_i), \tag{3}$$

with

$$\mathbf{S}_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{i} \mathbf{S}_i \exp(-i\mathbf{q} \cdot \mathbf{R}_i),$$

where N $(= N_1N_2N_3)$ is the total number of spins, and $\mathbf{S}_q^* = \mathbf{S}_{-q}$. The position vector $\mathbf{R}_i$ is expressed by

$$\mathbf{R}_i = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \ (n_1, n_2, n_3 \text{ are integers}),$$

where $n_1 = 0, 1, \cdots, N_1$, $n_2 = 0, 1, \cdots, N_2$, $n_3 = 0, 1, \cdots, N_3$, and $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are the fundamental lattice vectors. We also define the reciprocal lattice vector G by

$$G(h, k, l) = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \ (h, k, l \text{ are integers}),$$

where $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ are fundamental reciprocal lattice vectors and are given by

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]}, \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]}, \mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]},$$

with

$$[\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3] = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1) = \mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2).$$

Noting that

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = 2\pi, \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi, \mathbf{a}_3 \cdot \mathbf{b}_3 = 2\pi,$$

we have

$$\mathbf{G}(h, k, l) \cdot \mathbf{R}_i = 2\pi(n_1h + n_2k + n_3l) = 2\pi \times \text{integer}.$$

The periodic boundary condition for $\mathbf{S}_i$ leads to

$$\exp[i\mathbf{q}\cdot(N_1\mathbf{a}_1)] = 1, \exp[i\mathbf{q}\cdot(N_2\mathbf{a}_2)] = 1, \exp[i\mathbf{q}\cdot(N_3\mathbf{a}_3)] = 1.$$

This means that the wavevector $\mathbf{q}$ is given by

$$\mathbf{q} = q_1\mathbf{b}_1 + q_2\mathbf{b}_2 + q_3\mathbf{b}_3,$$

where

$$q_1 = \frac{m_1}{N_1}, q_2 = \frac{m_2}{N_2}, q_3 = \frac{m_3}{N_2}.$$

For convenience we assume that

$$-\frac{N_1}{2} \leq m_1 \leq \frac{N_1}{2}, -\frac{N_2}{2} \leq m_2 \leq \frac{N_2}{2}, -\frac{N_3}{2} \leq m_3 \leq \frac{N_3}{2},$$

corresponding to the first Brillouin zone. There are $N_1N_2N_3 = N$ wavevectors in the first Brillouin zone. The spin Hamiltonian is rewritten as

$$H = -\sum_{\mathbf{q}} J(\mathbf{q})\mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}}. \tag{4}$$

We look for the lowest minimum of Eq.(1) under the condition that

$$\mathbf{S}_i^2 = S^2 = \frac{1}{N} \sum_{\mathbf{q},\mathbf{q}'} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}'} \exp[i(\mathbf{q} - \mathbf{q}') \cdot \mathbf{R}_i], \tag{5}$$

for any i. Instead of this condition, we impose a milder condition

$$\begin{aligned} NS^2 &= \sum_i \mathbf{S}_i^2 = \frac{1}{N} \sum_i \sum_{\mathbf{q},\mathbf{q}'} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}'} \exp[i(\mathbf{q} - \mathbf{q}') \cdot R_i] \\ &= \sum_{\mathbf{q}} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}}, \end{aligned} \tag{6}$$