Spin configurations of the four-sublattice model on rectangular lattice

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ABSTRACT

The spin configurations of the four-sublattice model with seven exchange interaction parameters (four of them are taken as direct-exchange interactions, the other three as super-exchange interactions) on a two-dimensional rectangular lattice have been investigated using a matrix method. For the four sublattices, using the two sets of the exchange parameters, we obtain collinear and non-collinear spin configurations for the given propagation vectors in the ground and the first excited states. When $\mathbf{k}=\mathbf{0}$, spin configuration is collinear ferromagnetic mode in the ground state and collinear antiferromagnetic mode in the first excited state. When $\mathbf{k}=[0.5, 0.5]$, spin configurations are non-collinear, that is, canted structures.

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1. Introduction

At the beginning of 1961, the most general method, including the anisotropic couplings, was put forward by Bertaut [1–7]. Bertaut's matrix method enables possible magnetic modes associated with a given propagation vector. Moreover, the symmetry properties of crystal gain importance. When the chemical and magnetic cells are identical, symmetry properties of the results obtained are compatible with that of Villain's method [8]. From the other part, the results of this method also agreed with that of the group theory. The greatest advantage of this method is to consider fundamental interaction being isotropic classical Heisenberg and is also applicable when the chemical and magnetic cells are not identical. Moreover, isotropic terms as well as anisotropic terms can be expressed by a Hamiltonian of a second order and problem reduces to an eigenvalue problem. Solving this eigenvalue equation, one is able to find all possible magnetic configurations. The existence of the helical structures in solid solutions $x\mathrm{Fe_2O_3}(1-x)\,\mathrm{Cr_2O_3}$ [9] and in the spinel structure [10] can be explained by the matrix method. The solid solution $\mathrm{CrAs_{1-x}Sb_x}$ in which the collinear magnetic structure is observed by neutron diffraction is investigated by Kallel et al. [11]. They determined the stability regions using the matrix method and obtained the ferromagnetic and helical modes. Townsend et al. [12] deal with triangular-spin structure by the application of this method and predicted triangular-spin magnetic ordering for $\mathrm{KFe_3(OH)_6(SO_4)_2}$ and $\mathrm{KFe_3(OH)_6(CrO_4)_2}$. Darendelioğlu et al. [13] applied the two-dimensional orthorhombic lattice with four spins using macroscopic and microscopic (matrix) methods and determined that the four collinear modes are along the z-axis and the non-collinear modes are in the xy-plane of the two-dimensional orthorhombic lattice.

On the other hand, there are some other methods for magnetic structure determination. For example, using the Monte-Carlo simulation method, Hong et al. [14] investigated the spin configurations of two-dimensional ferromagnetic/antiferromagnetic systems. In order to investigate the different magnetic states corresponding to collinear and non-collinear spin configurations of $\mathrm{Mn_5Ge_3}$ compound, Stroppa et al. [15] performed fully unconstrained ab initio pseudo potential calculations within density functional theory. Yu et al. have given the phase diagram of the different spin configurations of a magnetic bilayer system consisting of two ferromagnetic layers, based on a phenomenological model [16]. Moreover, many researchers studied experimentally whether collinear and non-collinear structures exist in the normal spinel $\mathrm{ZnFe_2O_4}$ [17], in $\mathrm{MnFe_{2-x}Cr_xO_4}$ [18], in pure and impurity doped $\mathrm{Fe_3BO_6}$ [19], in multilayered Fe/Si films [20], in Fe–Zn metallic glasses [21], in BaCo [22], in $\varepsilon\text{-}\mathrm{Fe_xN}$ [23] and in $\mathrm{CeH_2/Fe}$ [24]. Furthermore, for the four-sublattice model, there are some interesting works within the linear–spin–wave theory [25–27].

In this paper, we will apply Bertaut's matrix method to the four-sublattice model on a rectangular lattice. Our aim is to find the possible spin configurations of the rectangular lattice with four-sublattice and seven exchange parameters using this theory. The outline of this paper is as follows. In Section 2, we start with a brief description of the matrix method and give the fundamental equations. In Section 3, we have determined possible spin configurations for the given $\mathbf{k}$-vectors and found collinear ferromagnetic, collinear antiferromagnetic and non-collinear (canted) spin configurations. Finally, Section 4 contains conclusions.

2. Matrix method

We derive spin configurations of the four sublattices on the rectangular lattice using the matrix method of Bertaut [7]. We will

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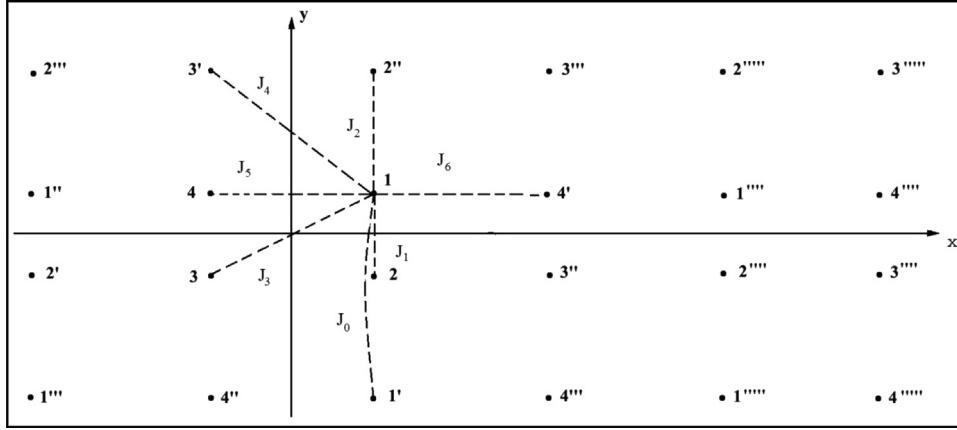E-mail address: gmert@selcuk.edu.tr (G. Mert).

Fig. 1. Two-dimensional rectangular lattice with the four sublattices and the magnetic interactions between neighboring ions.

Table 1
Computationally obtained eigenvalues and their eigenvectors for given **k**-vectors.

k-vectors	Exchange parameters	Eigenvalues	Eigenvectors
$\mathbf{k}_1 = [0, 0]$	S-I	$\lambda_1(\mathbf{k}_1) = 0.026$	$\mathbf{Q}_1(\mathbf{k}_1) = [-½\ \ ½\ \ ½\ \ -½]$
		$\lambda_2(\mathbf{k}_1) = -0.004$	$\mathbf{Q}_2(\mathbf{k}_1) = [½\ \ ½\ \ ½\ \ ½]$
		$\lambda_3(\mathbf{k}_1) = -0.010$	$\mathbf{Q}_3(\mathbf{k}_1) = [½\ \ ½\ \ ½\ \ ½]$
		$\lambda_4(\mathbf{k}_1) = -0.012$	$\mathbf{Q}_4(\mathbf{k}_1) = [½\ \ ½\ \ ½\ \ ½]$
	S-II	$\lambda_1(\mathbf{k}_1) = 0.038$	$\mathbf{Q}_1(\mathbf{k}_1) = [-½\ \ ½\ \ ½\ \ -½]$
		$\lambda_2(\mathbf{k}_1) = -0.078$	$\mathbf{Q}_2(\mathbf{k}_1) = [½\ \ ½\ \ ½\ \ ½]$
		$\lambda_3(\mathbf{k}_1) = 0.024$	$\mathbf{Q}_3(\mathbf{k}_1) = [½\ \ -½\ \ ½\ \ -½]$
		$\lambda_4(\mathbf{k}_1) = 0.016$	$\mathbf{Q}_4(\mathbf{k}_1) = [-½\ \ -½\ \ ½\ \ ½]$
$\mathbf{k}_2 = [0.5, 0.5]$	S-I	$\lambda_1(\mathbf{k}_2) = 0.08$	$\mathbf{Q}_1(\mathbf{k}_2) = [½\ \ ½\ \ ½\ \ ½]$
		$\lambda_2(\mathbf{k}_2) = -0.038$	$\mathbf{Q}_2(\mathbf{k}_2) = [½\ \ -½\ \ ½\ \ -½]$
		$\lambda_3(\mathbf{k}_2) = -0.018$	$\mathbf{Q}_3(\mathbf{k}_2) = [½\ \ -½\ \ -½\ \ ½]$
	S-II	$\lambda_4(\mathbf{k}_2) = -0.024$	$\mathbf{Q}_4(\mathbf{k}_2) = [½\ \ ½\ \ -½\ \ -½]$
		$\lambda_1(\mathbf{k}_2) = -0.002$	$\mathbf{Q}_1(\mathbf{k}_2) = [½\ \ -½\ \ ½\ \ -½]$
		$\lambda_2(\mathbf{k}_2) = -0.034$	$\mathbf{Q}_2(\mathbf{k}_2) = [-½\ \ -½\ \ ½\ \ ½]$
		$\lambda_3(\mathbf{k}_2) = 0.024$	$\mathbf{Q}_3(\mathbf{k}_2) = [-½\ \ ½\ \ ½\ \ -½]$
		$\lambda_4(\mathbf{k}_2) = 0.012$	$\mathbf{Q}_4(\mathbf{k}_2) = [½\ \ ½\ \ ½\ \ ½]$

Table 2
The corresponding phase angles for the ground and the first excited states.

k-vectors	Exchange parameters	Eigenvalues	Phase angles			
$\mathbf{k}_1 = [0, 0]$	S-I	$\lambda_4(\mathbf{k}_1) = -0.012$	$\varphi_1 = 0,$	$\varphi_2 = \pi,$	$\varphi_3 = 0,$	$\varphi_4 = \pi$
		$\lambda_3(\mathbf{k}_1) = -0.010$	$\varphi_1 = 0,$	$\varphi_2 = 0,$	$\varphi_3 = 0,$	$\varphi_4 = 0$
	S-II	$\lambda_2(\mathbf{k}_1) = -0.078$	$\varphi_1 = 0,$	$\varphi_2 = 0,$	$\varphi_3 = 0,$	$\varphi_4 = 0$
		$\lambda_4(\mathbf{k}_1) = 0.016$	$\varphi_1 = \pi,$	$\varphi_2 = \pi,$	$\varphi_3 = 0,$	$\varphi_4 = 0$
$\mathbf{k}_2 = [0.5, 0.5]$	S-I	$\lambda_2(\mathbf{k}_2) = -0.038$	$\varphi_1 = 0,$	$\varphi_2 = \pi,$	$\varphi_3 = 0,$	$\varphi_4 = \pi$
		$\lambda_4(\mathbf{k}_2) = -0.024$	$\varphi_1 = 0,$	$\varphi_2 = 0,$	$\varphi_3 = \pi,$	$\varphi_4 = \pi$
	S-II	$\lambda_2(\mathbf{k}_1) = -0.034$	$\varphi_1 = \pi,$	$\varphi_2 = \pi,$	$\varphi_3 = 0,$	$\varphi_4 = 0$
		$\lambda_1(\mathbf{k}_1) = -0.002$	$\varphi_1 = 0,$	$\varphi_2 = \pi,$	$\varphi_3 = 0,$	$\varphi_4 = \pi$

assume that there is a classical interaction of Heisenberg type between the spins. Hamiltonian is given by

$$H = -2\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where J_{ij} is the exchange integral between spins at $\mathbf{r}_i$ and $\mathbf{r}_j$. $\mathbf{S}_i$ is the spin vector at point $\mathbf{r}_i$.

Using the translational symmetry of the system, one obtains

$$\lambda_i \mathbf{S}_i(\mathbf{k}) = \sum_j J_{ij}(\mathbf{k})\mathbf{S}_j(\mathbf{k}), \tag{2}$$

where λ_i is a constant of proportionality, having the dimension of an energy. After a Fourier transformation, Eq. (2) can be written as a matrix equation:

$$(J(\mathbf{k}) - \lambda)\,\mathbf{S}(\mathbf{k}) = 0, \tag{3}$$

where λ is the diagonal matrix formed by the elements $\lambda_i \delta_{ij}$ ($i = 1,.., n$; n is the number of sublattices). $\mathbf{S}_i(\mathbf{k})$ is a column vector being the Fourier transformations of the $\mathbf{S}_i(\mathbf{r}_i)$

$$\mathbf{S}_i(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{r}_i}\mathbf{S}_i(\mathbf{r}_i)\exp(2\pi i\mathbf{k}\cdot\mathbf{r}_i), \tag{4}$$

$$\mathbf{S}_i(\mathbf{r}_i) = \frac{1}{N}\sum_{\mathbf{k}}\mathbf{S}_i(\mathbf{k})\exp(-2\pi i\mathbf{k}\cdot\mathbf{r}_i), \tag{5}$$

where N is the number of unit cells in the lattice. The hermitian interaction matrix $J(\mathbf{k})$ is the Fourier transformation of J_{ij} and

whose matrix elements are defined as follows:

$$J_{ij}(\mathbf{k}) = \sum_{\mathbf{r}_i} J_{ij}\exp[2\pi i\mathbf{k}\cdot(\mathbf{r}_{i0} - \mathbf{r}_j)], \tag{6}$$

where $\mathbf{r}_{i0}$ is a fixed reference point and the summation is over all $\mathbf{r}_j$ belonging to the same Bravais lattice j.

The expression of $\mathbf{S}_i(\mathbf{k})$ depended on phase is as follows:

$$\mathbf{S}_i(\mathbf{k}) = \tfrac{1}{2}(\hat{\mathbf{x}} + i\hat{\mathbf{y}})\exp(i\varphi_i), \tag{7}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are orthogonal unit vectors, ϕ_i is a phase angle of sublattice i. The angle between the two spins $\mathbf{S}_i(\mathbf{r}_i)$ and $\mathbf{S}_i(\mathbf{r}_i)$ in a one mode solution is given by

$$\Theta_{ij}(\mathbf{r}_1, \mathbf{r}_2) = 2\pi\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j) + (\varphi_i - \varphi_j). \tag{8}$$

The matrix $J(\mathbf{k})$ in Eq. (3) still depends on the atomic coordinates. With following transformation of eigenvectors:

$$\mathbf{Q}_i = \mathbf{S}_i(\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r}_{i0}), \tag{9}$$

one may construct a hermitian matrix $\eta(\mathbf{k})$ which does not depend on the atomic coordinates

$$(\eta(\mathbf{k}) - \lambda)\mathbf{Q} = 0. \tag{10}$$

In the case of only one propagation vector $\mathbf{k}$, the reference spins are simply given by

$$S(\mathbf{r}_{i0}) = \mathbf{Q}_i(\mathbf{k}) + \mathbf{Q}_i^*(\mathbf{k}), \tag{11}$$

$$S(\mathbf{r}_{i0}) = \mathbf{S}_i(\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r}_{i0}) + \mathbf{S}_i^*(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}_{i0}), \tag{12}$$

$$S(\mathbf{r}_{i0}) = \hat{\mathbf{x}}\,\cos(\mathbf{k}\cdot\mathbf{r}_{i0} + \varphi_i) + \hat{\mathbf{y}}\,\sin(\mathbf{k}\cdot\mathbf{r}_{i0} + \varphi_i). \tag{13}$$

This is the main equation in order to find spin directions for a given **k**-vector.