# Spin Configuration in a 2D- Orthorhombic Lattice With Symmetry Centers

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**Abstract:** The phase comparision method of E.F. Bertaut has been applied to the spin problem of two dimensional orthorhombic lattice with symmetry centers.The propagation vectors and the stability conditions have been obtained in the form of inequalities between the exchange constants. The eigenvalues have also been obtained in the non-parametric representation form and one establishes that it is impossible to express them in the parametric representation form.

**Key Words:** Spin Configuration, Exchange Constants, Orthorhombic Lattice

## Simetri Merkezli İki Boyutlu Ortorombik Bir Örgüde Spin Şekillenimleri

**Özet:** E. F. Bertaut' un Faz Mukayese Metodu iki boyutdaki simetri merkezli ortorombik örgüdeki spin proplemine uygulanmıştır.Yayılma vektörleri ve kararlılık koşulları değişim katsayıları arasındaki eşitsizlikler biçiminde ifade edilmiştir. Ayrıca özdeğerler de parametrik olmayan temsiller şeklinde elde edilerek bunların parametrik temsil şeklinde ifade etmenin mümkün olmadığı görülmüştür.

**Anahtar Kelimeler:** Spin Şekillenimi, Değişim Katsayıları, Ortorombik Örgü

## Introduction

The so called microscopic method (Matrix method) and macroscopic theory (Group theoretical method) developed by E.F. Bertaut [1] for studying spin configurations in ordered structures have applications of the mean field theory. According to the microscopic theory of Bertaut the magnetic ordering yields the following equation in the momentum space:

$$\zeta(\mathbf{k})\mathbf{T}(\mathbf{k}) = \lambda\mathbf{T}(\mathbf{k}) \tag{1}$$

where $\mathbf{T}(\mathbf{k})$ is a vector of n components $\mathbf{T}_i(\mathbf{k})$ (i =1,...,n) and the matrix $\zeta(\mathbf{k})$ is the Fourier transform of the isotropic spin-spin interactions. (In the presence of the anisotropy, this formalism can also be easily extended by making use of tensors.) $\mathbf{T}_j(\mathbf{k})$ in the above equation is given by

$$\mathbf{T}_j(\mathbf{k}) = \sum_{\mathbf{R}_j} \sigma_j(\mathbf{R}_j)\exp(2\pi i\mathbf{k}.\mathbf{R}_j). \tag{2}$$

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Structures  providing the minimum of the eigenvalue correspond to the stable configurations. In the case of  the existence of a **k**-vector different from zero, it is quite tedious to apply the microscopic method. But such a case could be solved more easily by the phase-comparison method of Bertaut [2] which does not need   an explicit knowledge of  eigenvalues and only uses the fact that the linear equations  under consideration  and belonging to a same  eigenvalue can be made either identical or conjugate. In this method one obtains the eigenvectors in a first stage. From their knowledge one gets the eigenvalues.

The above mentioned method will be used for the study of the spin configurations in the two-dimensional orthorhombic lattice which is decorated by spins as seen Figure 1.The reference spins are located at the points: $x,y(1)$; $x,\bar{y}(2)$; $\bar{x},\bar{y}(3)$; $\bar{x},y(4)$. One assumes that  the spins are axial vectors and have the same magnitudes. One  assume also that the spins interact with each other by means of  exchange interactions only. Let us define $J(i,j)$ as the exchange interaction constant between  the spin i and the spin j, located at **r**(i) and **r**(j) respectively. Just  the first nearest neighbours interactions between the sublattices  will only be taken into account and assume that there is no anisotropy at all between and within the sublattices.
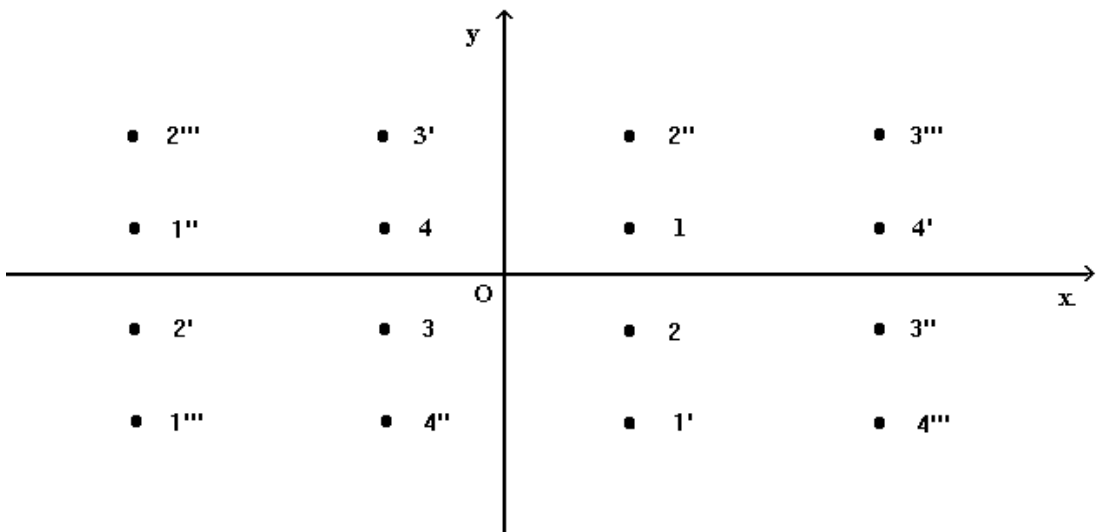


Figure 1. Two-dimensional Orthorhombic Lattice and Its  Sublattices.

**Theory**

The essential point of the method is that the  generalized Fourier transform of the exchange integral must be maximum [3]. The Fourier transform of the exchange integral is defined as follows:

$$\zeta_{ij} = \sum_{\mathbf{R}_j} J_{\mathbf{R}_i \mathbf{R}_j} \exp[2\pi i k \cdot (\mathbf{R}_i - \mathbf{R}_j)] .$$  (3)

where $J_{R_i R_j}$ is the exchange constant between spins at $R_i$ and $R_j$. This constant is positive for parallel spins (Ferromagnetism) and negative for antiparallel spins (Antiferromagnetism). Following Bertaut's matrix formalism, the above expression is evaluated by fixing $R_i$ and by summing on all spins of the atoms $R_j$ of lattice j which have the same $J_{R_i R_j}$ values. Therefore from eq (3) one has following coefficient of the interaction matrix in the case of isotropic exchange for the orthorhombic two dimensional lattice. The spin at x,y(1) has the following two near neighbours on lattice 2:x, $\bar{y}$ (2) and x,1-y(2'). The coefficient $\zeta_{12}$ of the matrix, according to eq (3) is

$$\zeta_{12} = 2 J_1 \cos 4\pi ky \ . \tag{4}$$

The spin at xy(1) has the following four nearest neighbours on lattice 3: $\bar{x}$, $\bar{y}$ (3);(1-x), $\bar{y}$ (3'); (1-x), (1-y)(3") and $\bar{x}$, (1-y)(3"). The elements of the interaction matrix, according to eq (3) is

$$\zeta_{13} = 2 J_3 \cos 2\pi( \ 2hx + 2ky \ )+ 2 J_3 \cos 2\pi( \ 2hx - 2ky \ ) \ . \tag{5}$$

Finally the spin at x,y(1) has the following two nearest neighbours 4: $\bar{x}$, y (4) and (1-x), y (4'). 

$$\zeta_{14}= 2 J_2 \cos 4\pi hx \tag{6}$$

where $J_1$ , $J_2$ and $J_3$ are the exchange constants defined above. When the propagation vector is different from zero, one has the following interaction matrix with generally complex elements $\zeta_{ij}$ Let us suppose that our points ( x, y ) are symmetry centers so that the complex part in eq (3) vanishes and the interaction matrix takes the following form:

$$\zeta(\mathbf{k}) = \begin{pmatrix} 0 & \zeta_{12} & \zeta_{13} & \zeta_{14} \\ \zeta_{12} & 0 & \zeta_{14} & \zeta_{13} \\ \zeta_{13} & \zeta_{14} & 0 & \zeta_{12} \\ \zeta_{14} & \zeta_{13} & \zeta_{12} & 0 \end{pmatrix} . \tag{7}$$

At this point, it is useful to replace the $\mathbf{T}_j(\mathbf{k})$ in eq (2) by new vectors $\mathbf{Q}(\mathbf{k})$ defined by

$$\mathbf{Q}_j(\mathbf{k}) = \mathbf{T}_j(\mathbf{k})\exp -i\mathbf{k}.\mathbf{r}_{j0} \ . \tag{8}$$

Defining a phase factor $Q_j$ of the form

$$Q_j = \exp -i\Psi_j \tag{9}$$

with $\Psi_j$ being the phase angle of the spin j, one has the following relations

$$\mathbf{S}(r_{j0}) = \mathbf{Q}_j(\mathbf{k}) + \mathbf{Q}_j(-\mathbf{k}) \tag{10}$$

$$\mathbf{S}(r_{j0}) = S_j(\mathbf{u}\cos\Psi_j + \mathbf{v}\sin\Psi_j) \tag{11}$$

Now let us find the eigenvalues of the matrix in eqn (7) using the phase comparison. For the sake of brevity denoted $\zeta_{12}$ by B, $\zeta_{13}$ by C and $\zeta_{14}$ by D .

$$\begin{pmatrix} -\lambda & B & C & D \\ B & -\lambda & D & C \\ C & D & -\lambda & B \\ D & C & B & -\lambda \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{pmatrix} = 0 \tag{12}$$

or

$$-\lambda + B\, Q_2\, Q_1^{-1} + C\, Q_3\, Q_4^{-1} + D\, Q_4\, Q_1^{-1} = 0 \tag{13}$$

$$-\lambda + B\, Q_1\, Q_2^{-1} + C\, Q_4\, Q_2^{-1} + D\, Q_3\, Q_2^{-1} = 0 \tag{14}$$

$$-\lambda + B\, Q_4\, Q_3^{-1} + C\, Q_1\, Q_3^{-1} + D\, Q_2\, Q_3^{-1} = 0 \tag{15}$$

$$-\lambda + B\, Q_3\, Q_4^{-1} + C\, Q_2\, Q_4^{-1} + D\, Q_1\, Q_4^{-1} = 0 \quad . \tag{16}$$

From the equivalence of eqs (13) and (15) , one has

$$Q_2\, Q_1^{-1} = Q_3\, Q_4^{-1} \; ; \; Q_3\, Q_4^{-1} = Q_2\, Q_4^{-1} \; ; \; Q_4\, Q_1^{-1} = Q_1\, Q_4^{-1} \tag{17}$$

From the third relation in eq (17) one observes that $Q_4\, Q_1^{-1}$ and $Q_1\, Q_4^{-1}$ are reals. From the remaining two equations it follows

$$\Psi_4 - \Psi_3 = \Psi_1 - \Psi_2 + 2\pi m \tag{18}$$
$$\Psi_1 - \Psi_3 = \Psi_4 - \Psi_2 + 2\pi n \quad .$$

Solving for $\Psi_3$ and $\Psi_4$ yields the following equations:

$$\Psi_3 = \Psi_2 - \pi(m+n) \tag{19}$$
$$\Psi_4 = \Psi_1 + \pi(m+n) \quad .$$

Depending on the parities of m and n there are two kinds of solution. Calling them a) and b) respectively.

a) m and n are of same parities

In this case one has

$$Q_3 = Q_2 \quad \text{and} \quad Q_4 = Q_1 \tag{20}$$

b) m and n are of different parities

In this case

$$Q'_3 = - Q'_2 \quad \text{and} \quad Q'_4 = - Q'_1 \tag{21}$$

are obtained. Substituting these Q values into the eq (13), one has the relation

$$\lambda - D = (B + C) Q_2 Q^{-1}_1 \ . \tag{22}$$

and using the condition that $\lambda$ - D is real, one comes to the conclusion that

$$Q_2 = \pm Q_1 \tag{23}$$

Substituting $Q_2$ values in eq (23) into the eq (22) the following eigenvalues are obtained in the form of non-parametric representation

$$\lambda_+ = B + C + D \tag{24}$$
$$\lambda_- = - B - C + D$$

for $Q_2 = Q_1$ and $Q_2 = - Q_1$ respectively. There is no parametric representation of the eigenvalues since the term B + C in eq (22) is real. This means that the phase angle $\Psi$ is equal to zero or integer multiples of $\pi$. One obtains the following eigenvalues for the primed values(that is for different parities of m and n) after having done some similar calculations :

$$\lambda'_+ = B - C + D \tag{25}$$
$$\lambda'_- = - B + C - D$$

The eigenvector matrix (Q) of the system, taking $Q_1 = Q$ and $Q'_1 = Q'$, becomes

$$\begin{pmatrix} Q & Q & Q & Q \\ -Q & Q & -Q & Q \\ -Q & Q & Q & -Q \\ Q & Q & -Q & -Q \end{pmatrix} . \tag{26}$$

The primed values are for different parities of m and n. The non - primed values are for the same parities of m and n. There are two columns for a given parity resulting from the equations $Q_1 = \pm Q_2$ and $Q'_1 = \pm Q'_2$ respectively.

From the phase relations (21) and (23) using the definition given by eq (9), one obtains the following reference spins where **u** has been chosen along the x-axis and **v** along the y-axis:

$$\sigma_1 = \mathbf{u}\cos\Psi_1 + \mathbf{v}\sin\Psi_1 \tag{27}$$
$$\sigma_2 = \mathbf{u}\cos\Psi_1 - \mathbf{v}\sin\Psi_1$$
$$\sigma_3 = \mathbf{u}\cos\Psi_1 - \mathbf{v}\sin\Psi_1$$
$$\sigma_4 = \mathbf{u}\cos\Psi_1 + \mathbf{v}\sin\Psi_1$$

In order to investigate the stability conditions it is sufficient to choose just one of the four eigenvalues obtained above, say $\lambda_+$ . Using the abbreviations H = h x and K = k y, one could write

$$\lambda_+ = 2J_1\cos 4\pi K + 2J_2 \cos 4\pi H + 2J_3 ( \cos 4\pi( H + K ) + \cos 4\pi ( H - K )) . \tag{28}$$

In order to find the possible **K**-propagation vectors from eq (28), one has to equate its derivatives with respect to H and K to zero,

$$\frac{\partial \lambda_+}{\partial H} = 0 \tag{29}$$

$$\frac{\partial \lambda_+}{\partial K} = 0$$

The doubly periodic function $\lambda_+ ( H, K )$ must have at least one minimum, one maximum and two saddle points. (In the case of three dimensions, say $\lambda_+ ( H, K, L )$ there should be at least one minimum, one maximum and six saddle points)

In order to obtain the stability conditions and the propagation vectors of the modes, one writes simply that $\lambda_+$ must be maximum (- $\lambda_+$ = H, exchange energy) i.e. the quadratic form, the coefficients of which are second derivatives of - $\lambda_+$ , must be definite positive. One can obtain the inequalities between the exchange constants as stability condition for all of the modes. The results are summarized in Table 1.

Table 1. Wave Vectors and Stability Conditions of Modes

| Wave vectors | Stability Conditions |
|---|---|
| [0 0] | $J_1 + 2J_3 \rangle 0$ ; $J_2 + 2J_3 \rangle 0$ ; $( J_1 + 2J_3 )( J_2 + 2J_3 ) \rangle 0$ |
| [1/4 0] | $J_1 - 2J_3 \rangle 0$ ; $J_2 + 2J_3 \langle 0$ ; $( J_1 - 2J_3 )( J_2 + 2J_3 ) \langle 0$ |
| [0 1/4] | $J_1 + 2J_3 \langle 0$ ; $J_2 - 2J_3 \rangle 0$ ; $( J_1 + 2J_3 )( J_2 - 2J_3 ) \langle 0$ |
| [1/4 1/4] | $J_1 - 2J_3 \langle 0$ ; $J_2 - 2J_3 \langle 0$ ; $( J_1 - 2J_3 )( J_2 - 2J_3 ) \rangle 0$ |
| [1 1/4] | $J_1 - 2J_3 \rangle 0$ ; $J_2 - 2J_3 \rangle 0$ ; $( J_1 - 2J_3 )( J_2 - 2J_3 ) \rangle 0$ |
| [1/4 1] | $J_1 - 2J_3 \rangle 0$ ; $J_2 + 2J_3 \langle 0$ ; $( J_1 - 2J_3 )( J_2 + 2J_3 ) \langle 0$ |

## Results

In this work, the eigenvalues and the corresponding eigenvectors of the interaction matrix have been determined  by the phase comparison method. Results are completely in agreement with our previous   results [4]. All of the eigenvalues have been obtained in the non-parametric representation form because of the fact that, the term B + C in eq (22) is real and it is impossible to split it into a real and an imaginary part.

The relations between the exchange constants have been determined  in the form of inequalities. .The importance of obtaining  inequalities between the exchange constants as  stability conditions  is that  it imposes further  boundary conditions  on the exchange constants' space and indicates the breakdown of a spin configuration for  some critical ratio of exchange constants, since from experiments one may only determine Curie or Néel  temperatures as linear combinations of exchange constants.

Finally among  the various  propagation vectors,  the obtained  one   corresponds  to the ferromagnetic configuration.

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