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THE EXISTENCE
OF A STABLE NONCOLLINEAR PHASE
IN A HEISENBERG MODEL
WITH COMPLEX STRUCTURE

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The study of Heisenberg magnets with complex structure is important for the understanding of magnetic properties of real substances [1]. In this letter we shall present some results of the mean-field analysis based on the model of two bilinearly coupled classical Heisenberg subsystems. The proper identification of the possible magnetic phases, their domain of existence and stability can be described by this fully isotropic model for a big class of magnetic materials, in which the different types of anisotropies are several orders smaller than the exchange interaction. The importance of purely exchange models for the description of phases and phase transitions in magnetic substances is well elucidated, for example, in [2], [3].

Our analysis is done with the help of the following microscopic hamiltonian:

$$H = -\frac{1}{2} \sum_{ij}^{2N} \left[ J_{ij}^{(1)} \mathbf{S}_i^{(1)} \cdot \mathbf{S}_j^{(1)} + J_{ij}^{(2)} \mathbf{S}_i^{(2)} \cdot \mathbf{S}_j^{(2)} + 2K_{ij} \mathbf{S}_i^{(1)} \cdot \mathbf{S}_j^{(2)} \right]. \tag{1}$$

The variables  $\mathbf{S}_{i}^{\alpha}$  are *n*-component classical spin vectors which obey the condition  $\left|\mathbf{S}_{i}^{(\alpha)}\right|=1$ ;  $(\alpha=1,2)$ . The dimensionless parameters,

$$J_{ij}^{\alpha} = \frac{\mathcal{J}_{ij}^{(\alpha)}}{T} , \quad K_{ij} = \frac{\mathcal{K}_{ij}}{T} , \qquad (2)$$

where T is the temperature, stand for the in-subsystems and intersubsystem exchange interactions, respectively. In the general case they are elements of  $(N \times N)$  matrix with N - the number of lattice sites in the subsystems.

The Ginzburg-Landau functional for the hamiltonian (1) is obtained in our previous paper [4] with the help of the Hubbard-Stratonovich transformation (HST). Somewhat different way of application of HST to the model (1) can be found in the book [5], where a RG analysis of the same model is done.

In the mean field calculations we neglect the spatial dependence of the order parameters and obtain the Landau free energy density in the form,

$$g \equiv \frac{G}{NT} = \frac{\tau_1}{2} \varphi_1^2 + \frac{\tau_2}{2} \varphi_2^2 + \frac{g_1}{4} (\varphi_1^2)^2 + \frac{g_2}{4} (\varphi_2^2)^2 + \frac{v}{2} \varphi_1^2 \varphi_2^2$$

$$+ v (\varphi_1 \cdot \varphi_2)^2 + w_1 \varphi_1^2 (\varphi_1 \cdot \varphi_2) + w_2 \varphi_2^2 (\varphi_1 \cdot \varphi_2) .$$
(3)

The n-component real-space vectors  $\varphi_i$ , (i=1,2), play the role of order parameters of the system. We shall consider only a positive in-subsystem exchange and the weak-coupling limit which means that the interaction between the subsystems is smaller than the in-subsystem interactions. As far as we do not take into account any magnetic anisotropies, we shall limit our considerations to magnetic substances with a cubic crystal structure as the bcc lattice with two different magnetic ions per unit cell. Under these conditions, the model (1) will describe two interpenetrating ferromagnetically ordered sublattices which interact either ferromagnetically or antiferromagnetically.

For a ferromagnetic in-subsystem exchange the coefficients in Eq. (3) will be expressed by the quantities  $S_0(\mathbf{k})$ ,  $S_1(\mathbf{k})$  and  $\lambda_{1,2}(\mathbf{k})$  for  $\mathbf{k}=0$ , where  $S_0(\mathbf{k})$  and  $S_1(\mathbf{k})$ , are the elements of the unitary matrix,  $\hat{S}$ , which diagonalizes the Ginzburg-Landau functional in  $\mathbf{k}$ -space and  $\lambda_{1,2}(\mathbf{k})$  are the respective eigenvalues. The matrix elements and eigenvalues are functions of the averaged over the nearest neighbours microscopic exchange parameters (2) denoted by  $J_1$ ,  $J_2$ , K, respectively (for details, see [4]). The Landau free energy depends on the number of order parameter components n through the parameter  $u=1/n^2(n+2)$  which enters linearly in all coefficients in front of the fourth order terms. The coefficients in front of the second order terms  $\tau_{1,2}$  are also functions of n;  $\tau_{1,2}=1-\lambda_{1,2}/n$ .

The initial hamiltonian, Eq. (1), is degenerate with respect to the rotations of all spins by one and the same angle and this degeneracy is preserved in the Landau free energy density, Eq. (3). That is why from the mean-field equations:

$$\frac{\partial g}{\partial \varphi_{1i}} = 0$$
,  $\frac{\partial g}{\partial \varphi_{2i}} = 0$ ,  $(i = 1, \dots, n)$ ,

we can find for n > 1, only the magnitudes of the vector order parameters  $\varphi_i$ , (i = 1, 2) and their mutual orientation. Our previous analysis shows that concerning the mutual orientation of vector order parameters, there are two possibilities, namely:

$$\cos(\varphi_1, \varphi_2) = \pm 1$$
 - collinear phases  $\cos(\varphi_1, \varphi_2) \neq \pm 1$  - noncollinear phases.

In the collinear case the system of equations for the magnitudes of vector order parameters  $\varphi_i$ , (i = 1, 2) can be solved only numerically and the results are described in details in [4].

The respective equations for the noncollinear phase can be treated analytically. Because of the degeneracy of Landau free energy density in a purely exchange approximation for n > 1, it is more appropriate to present  $\varphi_1$  and  $\varphi_2$  by the direction

proximation for n > 1, it is more appropriate to present  $\varphi_1$  and  $\varphi_2$  by the direction cosines  $\gamma_i$  and  $\alpha_i$  and their magnitudes  $\varphi_1 = \left(\sum_{i=1}^n \varphi_{1i}^2\right)^{1/2}$ ,  $\varphi_2 = \left(\sum_{i=1}^n \varphi_{2i}^2\right)^{1/2}$ , in the following way,

$$\varphi_{1i} = \varphi_1 \gamma_i, \quad \varphi_{2i} = \varphi_2 \alpha_i . \tag{4}$$

Then the Landau free energy density, Eq. (3) is rewritten with the help of Eq. (4) and afterwards minimized with respect to  $\alpha_i \gamma_i$ ,  $\varphi_1$  and  $\varphi_2$  under the conditions

$$\sum_{i=1}^{n} \alpha_i^2 = 1, \quad \sum_{i=1}^{n} \gamma_i^2 = 1.$$

The resulting mean field equation for  $\cos(\varphi_1, \varphi_2) = \sum_{i=1}^n \alpha_i \gamma_i$  will be,

$$2v\varphi_1\varphi_2\sum_{i=1}^n \alpha_i\gamma_i + w_1\varphi_1^2 + w_2\varphi_2^2 = 0.$$

It is obvious from the above expression that the cosine between the vector order parameters is well defined for  $\varphi_1 \neq 0$  and  $\varphi_2 \neq 0$ . The vector order parameters will be mutually perpendicular when  $w_1 = 0$ ,  $w_2 = 0$ . This is possible for equivalent sublattices because  $w_{1,2} \sim (J_1 - J_2)$ , but in this case the system of equations for  $\varphi_1$  and  $\varphi_2$  has a solution only when  $K \equiv 0$ , which means fully decoupled sublattices.

When  $J_1 \neq J_2$  the system of equations for  $\varphi_1$ ,  $\varphi_2$  is simple and can be solved directly,

$$\begin{split} \tau_1 + (g_1 - \frac{w_1^2}{v})\varphi_1^2 + (v - \frac{w_1 w_2}{v})\varphi_2^2 &= 0, \\ \tau_2 + (g_2 - \frac{w_2^2}{v})\varphi_2^2 + (v - \frac{w_1 w_2}{v})\varphi_1^2 &= 0. \end{split}$$

To understand the properties of the obtained magnetic phase we need the connection between the order parameter vectors  $\boldsymbol{\varphi}_i$ , (i=1,2), and the sublattice magnetizations,  $\boldsymbol{m}_i$ , (i=1,2)

$$egin{aligned} oldsymbol{m}_1 &= rac{S_0}{\lambda_1} oldsymbol{arphi}_1 - rac{S_1}{\lambda_2} oldsymbol{arphi}_2 \,, \ oldsymbol{m}_2 &= rac{S_1}{\lambda_1} oldsymbol{arphi}_1 + rac{S_0}{\lambda_2} oldsymbol{arphi}_2 \,. \end{aligned}$$

From the above expression we can find the magnitudes of the sublattice magnetizations and the angle  $\gamma$  between them. The requirements

$$|\cos \gamma| \le 1$$
 and  $|\sum_{i=1}^{n} \alpha_i \gamma_i| \le 1$ 

restrict the values of parameters  $J_1, J_2$  and K, for which the noncolliner phase can exist.

The analytical expressions for magnitudes of the sublattice magnetizations and  $\cos \gamma$  can be obtained straightforwardly after some algebra but they are very cumbersome, moreover, the temperature dependence of  $m_1$ ,  $m_2$  and  $\cos \gamma$  cannot be comprehended directly from formulae. For this reason we prefer to give a graphical presentation of our results. In order to compare the properties of the noncollinear and collinear phases, obtained previously, we shall rewrite the solutions for the noncollinear phase with the help of the dimensionless parameters, introduced in [4]:

$$x = \frac{T}{\mathcal{J}_1 + \mathcal{J}_2}, \quad \alpha = \frac{\mathcal{J}_1 - \mathcal{J}_2}{\mathcal{J}_1 + \mathcal{J}_2}, \quad \beta = \frac{2\mathcal{K}}{\mathcal{J}_1 + \mathcal{J}_2}.$$

The quantity x is called the reduced temperature;  $\alpha$  can be considered as a measure of the difference between the two sublattices. We assume that,  $\mathcal{J}_1 > \mathcal{J}_2$ , because the sublattices are symmetric with respect to the interchange  $1 \leftrightarrow 2$ ; then,  $0 < \alpha < 1$ .

The dimensionless intersublattice interaction,  $|\beta| < 1$ , which is a requirement of the weak-coupling limit

 $\mathcal{J}_1\mathcal{J}_2-\mathcal{K}^2>0.$ 

In Fig. 1 the variation of  $\cos \gamma$  with the reduced temperature x is depicted for a fixed value of  $\alpha$  and three different values of  $\beta$ . The behaviour of  $\cos \gamma$  is essentially different for different values of the relation  $\alpha/\beta$ . When  $\alpha \geq \beta$ , the noncollinear phase is metastable in the whole domain of its existence and  $\cos(\gamma) < 1$ , including the phase transition point. In the opposite case, i.e,  $\alpha < \beta$ , the noncolliner phase becomes the most stable phase in the temperature interval  $x_n < x \leq x^*$ , where  $x^*$  is the transition temperature of the noncollinear phase and  $x_n$  is the temperature, below which the noncollinear phase does not exist. For  $\beta = 0.003$ , the angle between the sublattice magnetizations vary from zero at  $x^*$  to  $\sim 68^\circ$  at  $x_n$ . When  $\beta$  grows (see the curve for  $\beta = 0.005$ ) the domain of the existence for the noncollinear ferrimagnetic phase becomes more narrow and for  $\beta \sim 0.0056$  it does not exist.

The calculations show that in the region of stability of the noncollinear phase the magnetization  $M=m_1+m_2$  is perpendicular to the staggered magnetization  $L=m_1-m_2$ . This is the condition for the existence and stability of a noncollinear ferrimagnetic phase, derived on the basis of a symmetry group analysis by Andreev and Marchenko [6].

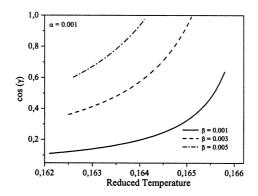


Figure 1: The temperature dependence of  $\cos \gamma$  for  $n=3,~\alpha=0.001$  and different values of the parameter  $\beta$ 

In Fig. 2 and Fig. 3 we compare the Landau free energy density as a function of the reduced temperature x for all magnetic phases we have found (collinear and noncollinear). The phase with the highest transition temperature, denoted by S in Figs. 2, 3, has a collinear ferrimagnetic structure with a compensation point at lower temperatures. It is stable and occurs through a second order phase transition. The symbols for the high- and low-temperature metastable collinear phases are

 $M_i$ , i = 1, 2, respectively.  $M_3$  is a collinear metastable phase, which occurs by a second order phase transition, not given in [4]. The Landau energy density of the noncollinear phase is denoted by New.

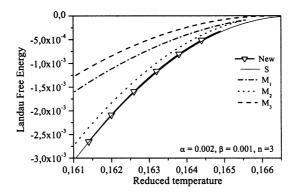


Figure 2: The temperature dependence of Landau free energy density for  $\alpha > \beta$ 

For  $\alpha > \beta$  the noncollinear phase has an energy slightly higher than the stable collinear phase - Fig. 2. When the difference between the interaction in the sublattices becomes smaller than the intersublattice interaction, the noncollinear phase has lower energy than the S-phase in the whole domain of its existence - Fig. 3.

We can argue that with the decrease of the temperature the system orders by a second order phase transition in the stable collinear ferrimagnetic phase and with the further lowering of temperature a second phase transition occurs and a new ordered noncollinear phase appears. At lower temperatures the noncollinear phase ceases to exist. It is obvious from the above figures that the domain of existence and stability of the noncollinear phase is very narrow and it can occur only for magnetic substances, in which the following relation between the averaged microscopic exchange parameters holds true:

$$(\mathcal{J}_1 - \mathcal{J}_2) < \mathcal{K} < \sqrt{\mathcal{J}_1 \mathcal{J}_2}$$
.

Up to now we have considered only the ferromagnetic exchange between the sublattices ( $\beta > 0$ ). As the calculations show the respective noncollinear phase for  $\beta < 0$ , i.e., for an antiferromagnetic coupling, exhibits a similar temperature behaviour as the ferrimagnetic noncollinear phase described above.

We did not study the noncollinear phase in the general case of n-component order parameters. The above calculations are made for n=3 which is the most interesting case up to our opinion. The analysis shows that for n=2 the domain of existence of the noncollinear phase is very tiny and we did not find values of the parameters  $\alpha$  and  $\beta$ , for which it can be stable.

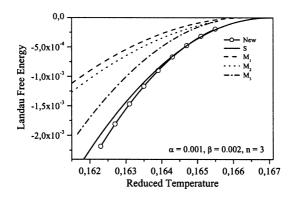


Figure 3: The temperature dependence of Landau free energy density for  $\alpha < \beta$ 

The difference between the energies of the stable collinear ferrimagnetic and the noncollinear ferrimagnetic phases is very small. In the real magnetic substances even a small anisotropic interaction may change the above described picture, but this problem needs a separate investigation.

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Шопова Д. В., Бояджиев Т. Л. Существование устойчивой неколлинеарной фазы в модели Гейзенберга сложной структуры E17-2002-280

Анализируются свойства неколлинеарной магнитной фазы, полученной в приближении среднего поля для двух связанных подсистем Гейзенберга. Область существования и устойчивости фазы довольно узкая и зависит от соотношения между усредненными по близким «соседям» микроскопическими обменными параметрами.

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Shopova D. V., Boyadjiev T. L. The Existence of a Stable Noncollinear Phase in a Heisenberg Model with Complex Structure E17-2002-280

We have analyzed the properties of a noncollinear magnetic phase obtained in the mean-field analysis of the model of two coupled Heisenberg subsystems. The domain of its existence and stability is narrow and depends on the ratio between the microscopic exchange parameters averaged over the nearest neighbours.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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