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The influence of the external field on phase states of a spin nematic with „easy-axis“ single-ion anisotropy

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The study has investigated the influence of the external magnetic field on the phase states of the spin nematic with „easy-axis“ single-ion anisotropy in the external magnetic field. We have considered a case of predominant biquadratic exchange interaction. The system is studied in two possible geometries: a field parallel to the anisotropy axis and a field perpendicular to the anisotropy axis. It is shown that in both the cases an axial nematic phase is realized in the system, but values of the fields of an axial nematic-paramagnetic state transition are different.

Keywords: spin nematic; „easy-axis“ single-ion anisotropy; external field; quadrupole ellipsoid.

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1. Introduction

The state of the spin nematic is one of the most unusual states of magnetic-ordered structures. Standard magnetic ordering is related to disturbance of time reversal symmetry [1,2], whereas in the spin nematic spontaneous disturbance of rotational symmetry is determined by multipole spin correlators that are average, i.e. different-node (or one-node) ones [3–22]. Usually, properties of the spin nematics are studied in case of no external field. At this, a question arises: will the nematic phase be stable when the external magnetic field is switched on? The influence of the magnetic field on stability of the nematic states is actively studied in magnetics with the magnetic-ion spin $S = 1/2$, in which the nematic state is characterized by different-node spin averages [23–34]. However, the influence of the magnetic field on the phases states of a non-Heisenberg magnetic with biquadratic exchange interaction results in new unusual outcomes. Thus, it was shown in the study [35] that both in the isotropic as well as the spin nematic with single-ion anisotropy the stable nematic state is realized. At the same time, the external magnetic field significantly affects a geometric image of this state in spin space. Thus, without the external field, the geometric image of the nematic state in spin space is a uniaxial ellipsoid (an infinitely thin disk), whereas switching on the field transforms the quadrupole ellipsoid into a two-axis ellipsoid. Besides, it was shown in the study [36] that in a ferromagnetic with high biquadratic exchange interaction and single-ion anisotropy of the „easy-plane“ type, presence of the external magnetic field perpendicular to the basal plane results in realization of an „angular“ nematic phase, in which the quadrupole two-axis ellipsoids are oriented at a certain angle to a quantization axis, i.e. results in realization of a new phase state — the „angular“ nematic

phase. Origination of this state is related to presence of easy-plane anisotropy that results in an effect of quantum spin reduction [37] and of the external magnetic field. A question arises: will it be energetically favorable to realize this „angular“ nematic phase in the easy-axis non-Heisenberg ferromagnetic that is in the external field orthogonal to the easy axis?

Thus, the aim of the present study is to investigate the phase states of the non-Heisenberg ferromagnetic with high biquadratic exchange interaction and single-ion anisotropy of the „easy-axis“ type, which is in the external magnetic field.

2. Non-Heisenberg anisotropic ferromagnetic in the longitudinal magnetic field

A studied model is considered to be a ferromagnetic with the magnetic-ion spin $S = 1$, whose exchange Hamiltonian takes into account both Heisenberg exchange and biquadratic exchange as well. Besides, the studied system has single-ion anisotropy of the „easy-axis“ type and is in the external magnetic field parallel to an easy-magnetization axis. The Hamiltonian of this ferromagnetic can be represented as follows:

$$\begin{aligned} \mathcal{H} = & -H \sum_n S_n^z - \beta \sum_n (S_n^z)^2 \\ & - \frac{1}{2} \sum_{n_1 \neq n_2} \left[J(n - n') (\mathbf{S}_n \mathbf{S}_{n'}) + K(n - n') (\mathbf{S}_n \mathbf{S}_{n'})^2 \right], \end{aligned} \quad (1)$$

where J, K — the constants of bilinear and biquadratic exchange interactions, $\beta > 0$ — the constant of single-ion anisotropy of the „easy-axis“ type, H — the external

field in energy units. Further on, we will consider only a case of high biquadratic exchange interaction $K > J$ and it is assumed that it is considered at low temperatures, i.e. $T \rightarrow 0$.

Before considering the influence of the external field on the state of the anisotropic spin nematic, we consider a behavior of the system when $H = 0$ [14]. As shown in the studies [12,16,17,19–21], in the case of high biquadratic exchange the nematic state is realized in the system, which is described by the following order parameters:

$$\langle S^z \rangle = \cos 2\alpha, \quad q_2^0 = 3\langle (S^z)^2 \rangle - S(S+1),$$

$$q_2^2 = \langle (S^x)^2 \rangle - \langle (S^y)^2 \rangle = \sin 2\alpha,$$

where α is a parameter of a generalized $u-v$ transformation [38], which in case of no external field can take the value $\pm\pi/4$. Thus, in the considered case the order parameters that determine the nematic state are as follows:

$$\langle S^z \rangle = 0, \quad q_2^0 = 1, \quad q_2^2 = \pm 1. \quad (2)$$

It follows from the relationships (2) that

$$\langle (S^z)^2 \rangle = 1, \quad \langle (S^x)^2 \rangle = 1, \quad \langle (S^y)^2 \rangle = 0,$$

if $\alpha = \pi/4$; or

$$\langle (S^z)^2 \rangle = 1, \quad \langle (S^x)^2 \rangle = 0, \quad \langle (S^y)^2 \rangle = 1,$$

if $\alpha = -\pi/4$. Thus, the geometric image in spin space of the nematic state of the anisotropic spin nematic with „easy-axis“ anisotropy is a uniaxial ellipsoid (an infinitely thin disk) that is oriented either in the ZOY plane ($\alpha = \pi/4$) or in the ZOY plane ($\alpha = -\pi/4$). At the same time, the ground state energy in both the cases is the same and is

$$E_{gs} = -\frac{K_0}{3} - \beta,$$

while ground state vectors are as follows:

$$|\psi_{gs}\rangle = \frac{|1\rangle + |-1\rangle}{\sqrt{2}} \quad (\alpha = \pi/4);$$

$$|\psi_{gs}\rangle = \frac{|1\rangle - |-1\rangle}{\sqrt{2}} \quad (\alpha = -\pi/4).$$

Consequently, the nematic state when $H = 0$ is degenerate in orientation of the quadrupole ellipsoids in spin space relative to the easy-magnetization axis, i.e. the axis OZ.

When switching on the external field parallel to the anisotropy axis, a nonzero magnetic moment originates, i.e. $\langle S^z \rangle \neq 0$, wherein its value is less than a nominal value of the magnetic-ion spin. In this case, the ground state energy is:

$$E_{gs} = -\frac{K_0}{3} - \beta - H \cos 2\alpha + \frac{1}{2} (K_0 - J_0) \cos^2 2\alpha, \quad (3)$$

while the order parameters take the form:

$$\langle S^z \rangle = \cos 2\alpha, \quad q_2^0 = 1, \quad q_2^2 = \sin 2\alpha, \quad (4)$$

where

$$\langle (S^x)^2 \rangle = \frac{1}{2} (1 + \sin 2\alpha);$$

$$\langle (S^y)^2 \rangle = \frac{1}{2} (1 - \sin 2\alpha); \quad \langle (S^z)^2 \rangle = 1. \quad (5)$$

Since we consider the behavior of the system at the low temperatures ($T \rightarrow 0$), then an expression for the ground state energy (3) determines a density of free energy of the studied magnetic. The density of free energy is analyzed to show that

$$\cos 2\alpha = \langle S^z \rangle = \frac{H}{K_0 - J_0},$$

i.e. with the fields that are less than the critical one ($H_c < K_0 - J_0$), a so-called axial nematic is realized in the spin nematic with easy-axis single-ion anisotropy, whose geometric image in spin space, as follows from the relationships (5), is a two-axis ellipsoid, whose main axis is parallel to the axis OZ, i.e. parallel both to the direction of the external field and the easy-magnetization axis as well.

With the fields that exceed H_c , the order parameters take the following form:

$$\langle S^z \rangle = 1, \quad q_2^0 = 1, \quad q_2^2 = 0,$$

and the magnetic transits into the paramagnetic state.

3. Non-Heisenberg anisotropic ferromagnetic in the transverse magnetic field

Now we consider a behavior of the easy-axis spin nematic in the transverse external field perpendicular to the easy-magnetization axis. For certainty, we assume that the magnetic field is parallel to the axis OZ and easy-axis anisotropy is oriented along the axis OX. As above, it is assumed that the magnetic-ion spin $S = 1$, the temperatures are low and the constant of biquadratic exchange interaction exceeds the constant of bilinear exchange, i.e. $K > J$. The magnetic Hamiltonian in this case is as follows:

$$\begin{aligned} \mathcal{H} = & -H \sum_n S_n^z - \beta \sum_n (S_n^x)^2 \\ & - \frac{1}{2} \sum_{n_1 \neq n_2} \left[J(n - n') (\mathbf{S}_n \mathbf{S}_{n'}) + K(n - n') (\mathbf{S}_n \mathbf{S}_{n'})^2 \right]. \end{aligned} \quad (6)$$

Switching on the external field will result in origination of the nonzero magnetic moment, whose orientation and value will be determined by competition of the external field and constitutive parameters of the system, in particular, single-ion anisotropy. It can be expected that in this geometry the so-called „angular“ nematic phase can be realized, as observed in the easy-plane spin nematic (see, for example, the study [36]). Consequently, it can be assumed that the magnetic moment that originates under effect of the magnetic field is oriented at a certain angle θ to the axis OZ.

For certainty, we will believe that the magnetic moment is in the ZOY plane. Using a unitary transformation

$$\mathcal{H}(\theta) = U\mathcal{H}U^\dagger, \quad U(\theta) = \prod_n \exp[i\theta S_n^y]$$

we will go over to an intrinsic system of coordinates at each node, in which the axis OZ coincides with a direction of the average magnetic moment. In the intrinsic system of coordinates, the ground state energy that coincides with the density of free energy in case of the low temperatures, takes the form:

$$E_{gr,st} = -H \cos \theta \cos 2\alpha + \frac{1}{2} (K_0 - J_0) \cos^2 2\alpha + \frac{\beta}{2} \cos^2 \theta (1 - \sin 2\alpha). \quad (7)$$

Here, as above, α is a parameter of the $u-v$ transformation.

By minimizing the density of free energy (7) by the parameters θ and α , we obtain a relationship of these parameters with the constitutive parameters of the magnetic:

$$\cos \theta = \frac{H}{\beta} \frac{\cos 2\alpha}{1 - \sin 2\alpha}, \quad \sin 2\alpha = -\frac{H^2}{2\beta(K_0 - J_0)}. \quad (8)$$

Using the relationships (8) as well as taking into account that in the intrinsic system of coordinates $\cos 2\alpha = \langle S^z \rangle$, we obtain

$$\langle S^z \rangle = \left(\frac{\beta}{H} + \frac{H}{2(K_0 - J_0)} \right) \cos \theta. \quad (9)$$

It follows from analysis of the expression (9) that the average value of the magnetic moment decreases with an increase of the value of the magnetic field, since the first summand decreases with the increase of the field as a hyperbole (at the fixed β, θ), while the second summand increases as a linear function. This behavior of the average values of the magnetic moment indicates that unlike the easy-plane nematic [36], the „angular“ phase is not realized in this case, but the axial nematic phase originates, in which the nonzero magnetic moment is parallel to the external field, while the order parameters are determined by the relationships (4). At the same time, the average magnetic moment increases with the increase of the field, while the quadrupole ellipsoid, as follows from an explicit form of the one-node correlators

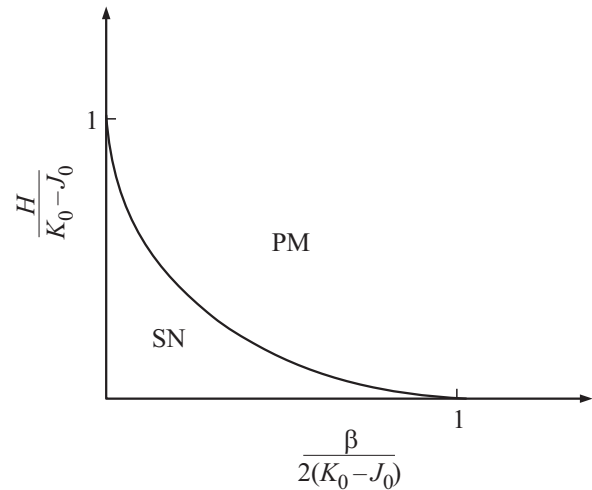
$$\langle (S^z)^2 \rangle = 1,$$

$$\langle (S^y)^2 \rangle = \frac{1}{2} (1 - \sin 2\alpha), \quad \langle (S^x)^2 \rangle = \frac{1}{2} (1 + \sin 2\alpha),$$

is transformed into the two-axis ellipsoid, whose main axis is oriented along the magnetic field.

In this phase, the ground state energy is:

$$E_{gr,st} = -H \cos 2\alpha + \frac{1}{2} (K_0 - J_0) \cos^2 2\alpha + \frac{\beta}{2} (1 - \sin 2\alpha). \quad (10)$$



Phase diagram of the spin nematic with „easy-axis“ anisotropy in the transverse magnetic field.

while the ground state wave vector is as follows: $|\psi_{gr,st}\rangle = \cos \alpha |1\rangle + \sin \alpha |-1\rangle$.

Since we consider the system at the low temperatures, then the ground state energy (when $T \rightarrow 0$) determines the density of free energy, whose parameter minimization allows obtaining the following equation for this parameter:

$$H \sin 2\alpha - (K_0 - J_0) \sin 2\alpha \cos 2\alpha + \frac{\beta}{2} \cos 2\alpha = 0.$$

After simple mathematical transformations this equation can be reduced to the following form:

$$\left(\frac{H}{K_0 - J_0} \right)^{2/3} + \left(\frac{\beta}{2(K_0 - J_0)} \right)^{2/3} = 1. \quad (11)$$

Generally, the equation (11) describes a closed curve (astroid) in variables

$$\frac{H}{K_0 - J_0}, \quad \frac{\beta}{2(K_0 - J_0)}$$

(see the study [1]). In the considered case the equation (11) describes only a part of the astroid, since all the parameters of (11) are positive, i.e. it is the part of the astroid, which is in the first quadrant. Besides, the equation (11) allows determining a field of a transition between the axial nematic phase characterized by the order parameters (4) and the paramagnetic state characterized by the order parameters

$$\langle S^z \rangle = 1, \quad q_2^0 = 1, \quad q_2^2 = 0.$$

A value of the critical field is determined as follows:

$$H_c = (K_0 - J_0) \left[1 - \left(\frac{\beta}{2(K_0 - J_0)} \right)^{2/3} \right]^{3/2}.$$

Thus, when $H < H_c$ the axial nematic state is realized, and when $H > H_c$ the paramagnetic phase is realized. Graphically, it can be presented as follows (see the figure).

4. Conclusion

What is the reason of such a striking difference between models that seem to be very close to each other: the spin nematic with „easy-plane“ anisotropy in the transverse field and the spin nematic with „easy-axis“ anisotropy in the transverse field as well?

In order to understand the resulting differences in the behavior of the magnetics with single-ion anisotropy „easy axis“ and „easy plane“ in the external magnetic field, we turn to consideration of the situation without the external field. As shown in the study [36], when $H = 0$ and biquadratic exchange interaction is high, the nematic state with $\langle S \rangle = 0$ is realized in the magnetic. At the same time, single-ion anisotropy of the „easy-plane“ type orients the uniaxial quadrupole ellipsoid (the infinitely thin disk) in the basal plane, i.e. creates effective anisotropy of the quadrupole order parameters. When switching on the external magnetic field perpendicular to the basal plane, there is competition between effective anisotropy and the magnetic field, thereby resulting in realization of the „angular“ nematic phase. In the case that is considered in the present study, i.e. of the spin nematic with „easy-axis“ anisotropy, when $H = 0$ the nematic state with $\langle S \rangle = 0$ is also realized, but the quadrupole ellipsoid (of the infinitely thin disk) is formed either in the XOZ plane or the ZOY plane. The external field that is switched on perpendicular to the anisotropy axis turns out to be in the plane of the uniaxial ellipsoid. It means that there is no competition between effective anisotropy of the quadrupole order parameters and the external field. Consequently, when switching on the external field oriented parallel to the axis OZ , there is the nonzero magnetic moment oriented along the magnetic field ($0 < \langle S^z \rangle < 1$) and the quadrupole two-axis ellipsoid is oriented so that its main axis is parallel to the axis OZ , too. Thus, in our considered case, when $H \neq 0$ and biquadratic exchange interaction is high, the „angular“ nematic phase is not realized, but the axial-nematic state originates.

Thus, it can be stated that symmetrical properties of the spin nematic with „easy-axis“ anisotropy and the spin nematic with „easy-plane“ anisotropy are different.

Conflict of interest

The authors declare that they have no conflict of interest.

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