ISSN 0021-3640, JETP Letters, 2017, Vol. 106, No. 1, pp. 30–34. © Pleiades Publishing, Inc., 2017.
Original Russian Text © S.N. Martynov, V.I. Tugarinov, 2017, published in Pis'ma v Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki, 2017, Vol. 106, No. 1, pp. 34–38.

CONDENSED MATTER

Phase Diagram of the Ground State of a Classical Anisotropic Frustrated Ferromagnet

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Received May 23, 2017

The phase diagram of the ground state is obtained for the one-dimensional easy-axis model of classical spins coupled by ferromagnetic and antiferromagnetic exchanges between nearest and next-nearest neighbors, respectively. The parameters of the incommensurate magnetic structure with a variable step (soliton lattice) are calculated in the mean field approximation from the condition of the collinearity of spins to the effective exchange fields in the continuous approximation. The ground state of the soliton lattice and interfaces between soliton and collinear (ferromagnetic and "up–up–down–down") phases are determined by the numerical minimization of the average energy over the initial angular velocity of spins.

DOI: 10.1134/S0021364017130124

In recent decades, frustrated magnets have caused ever-growing interest owing to the vast variety of unusual states and their magnetic properties [1]. A large number of works were devoted to the one-dimensional frustrated Heisenberg model, where the combination of the frustration of exchange interactions and strong quantum fluctuations leads to different states without any long-range magnetic order even at zero temperature and to quantum phase transitions between them [2–9]. In real quasi-low-dimensional magnetic crystals, the long-range magnetic order is established owing to weaker three-dimensional interactions [10]. The application of quantum approaches in the calculation of three-dimensional models is accompanied by the considerable increase in complications of calculations. As a starting point of calculations, one often uses the results of the consideration of corresponding classical models, which makes it possible to considerably narrow the region of search for solutions. Solutions of simple models with classical spins describe magnetically ordered phases in the mean field approximation qualitatively correctly and can easily be generalized to cases of an arbitrary dimension.

The ground state of the one-dimensional frustrated anisotropic Heisenberg model

$$H = J_1\sum_i(\mathbf{S}_i\mathbf{S}_{i+1} + \delta_1 S_i^z S_{i+1}^z) + J_2\sum_i(\mathbf{S}_i\mathbf{S}_{i+2} + \delta_2 S_i^z S_{i+2}^z), \quad (1)$$

$$J_1 < 0, \quad J_2 > 0, \quad \delta_{1,2} > 0,$$

where $J_2 > 0$ is the antiferromagnetic exchange with next-nearest magnetic neighbors, is determined by the sign of the exchange with the nearest neighbors J_1, the ratio of exchanges $R = J_2/J_1$, and their anisotropy δ_1 and δ_2.

For the case of the ferromagnetic exchange $J_1 < 0$, frustration leads to the appearance of different states with and without the long-range magnetic order [7–9, 11–13]. Interest in such magnetic materials is due to the increased number of synthesized chain copper compounds [14, 15] and to actively studied multiferroic properties of the latter [16, 17]. In the model given by Eq. (1) with classical vector spins, the easy plane exchange anisotropy ($\delta_1, \delta_2 < 0$) at $|R| > 1/4$ leads to a helix with the polarization plane coinciding with the easy plane and a constant step (the angle between the nearest spins φ). The latter maximally simplifies the calculation of its value, since all spins are in the equivalent relative surrounding. The minimization of the energy over the helix step leads to the standard result $\cos\varphi = -1/4R$. In the case of the easy-axis anisotropy, the classical solution of the model (1) becomes fundamentally more complicated. The helicoid with the polarization plane containing the easy axis has the minimum energy [18]. The exchange fields acting on a spin depend on the angle between its direction and the anisotropy axis z. As a result, the helicoid step becomes variable; i.e., a soliton lattice is formed. For its description, it is necessary to use the continuous approximation where the change in the orientation angle of spins is represented in the form of an analytic function of the coordinate $\theta(r_i)$. In such an approach, the determination of the equilibrium orientation of spins (of the form of the function $\theta(r_i)$) is reduced to the minimization of the integral of the magnetic energy density [18] or the expansion of the Ginzburg–Landau thermodynamic potential at a finite temperature [19]. This leads to the nonlinear Euler–Lagrange differential equation of at least the fourth order, the only way to solve which remains the substitution of trial harmonic functions (harmonics of the solution for the uniform helix). An essential restriction of the minimization procedure is also the accompanying replacement of trigonometric functions of the derivatives of the orientation angle of spins for the arguments.

We proposed an alternative method of the calculation of soliton lattice parameters in the model (1) in [20]. It is based on the principle of the collinearity of the average values of spins to the total effective fields at each lattice site. The principle was used earlier for the calculation of plane and conic incommensurate magnetic structures in a two-subsystem magnetic material on a discrete lattice [21–23] and was substantiated by Kaplan and Menyuk within the Lagrangian formalism in [24]. It allows avoiding nonphysical states and determining the ground and excited states of the system of spins. In the general case, with the continuous approach, the initial equation of vanishing of the field component transverse to the direction of the spin at the site is an equation for the series of even and odd derivatives of the orientation angle of the spin. Series of even derivatives ($\theta^{(2n)}$) determining the nonlinearity of solutions are proportional to the anisotropy. At the small nonlinearity ($\theta'' \ll 1$), this equation becomes an autonomous first-order differential equation with respect to the square of the angular velocity θ' and allows the solution in quadratures. The explicit form of the dependence θ' on the angle θ and the initial condition θ'_0 makes it possible to numerically minimize the average energy per spin in the soliton lattice over the initial condition, thus determining the ground state. This work is aimed at the determination of the phase diagram of the ground state of the classical frustrated ferromagnet (1) at $\delta_1 = \delta_2 = \delta > 0$ within this approach.

In the mean field approximation, all spins at $T = 0$ have the same length $S = 1$ and their orientation in the plane containing the easy axis of the anisotropy is determined by the total exchange field from neighboring spins. Field components along the anisotropy axis z and the orthogonal axis x in units of the ferromagnetic exchange J_1 have the form

$$\begin{aligned} h_z &= (1+\delta)h_z^0, \\ h_z^0 &= \frac{1}{2}\Big(\cos\theta_{i+1} + \cos\theta_{i-1} \\ &\quad + R(\cos\theta_{i+2} + \cos\theta_{i-2})\Big), \\ h_x &= \frac{1}{2}\Big(\sin\theta_{i+1} + \sin\theta_{i-1} \\ &\quad + R(\sin\theta_{i+2} + \sin\theta_{i-2})\Big), \end{aligned} \tag{2}$$

where h_z^0 is the z component of the exchange field without anisotropy and $\theta_{i\pm1,2}$ are the angles of the orientation of neighboring spins with respect to the anisotropy axis.

The transition to the continuous description is carried out by expanding the angles of neighboring spins in a Taylor series near the angle of the ith spin

$$\begin{aligned} \theta_i &= \theta, \\ \theta_{i\pm1} &= \theta \pm \Sigma_{11} + \Sigma_{12}, \\ \theta_{i\pm2} &= \theta \pm \Sigma_{21} + \Sigma_{22}, \end{aligned} \tag{3}$$

where $\Sigma_{\alpha\beta}$ are sums over odd and even derivatives of the variable θ,

$$\Sigma_{11} = \sum_{n=1}^{\infty} \frac{\theta^{(2n-1)}}{(2n-1)!}, \quad \Sigma_{22} = \sum_{n=1}^{\infty} \frac{2^{2n}\theta^{(2n)}}{(2n)!},$$

$$\Sigma_{12} = \sum_{n=1}^{\infty} \frac{\theta^{(2n)}}{(2n)!}, \quad \Sigma_{21} = \sum_{n=1}^{\infty} \frac{2^{2n-1}\theta^{(2n-1)}}{(2n-1)!}.$$

Here and below, the lattice constant is taken as unity. After the substitution of expansions (3), the field components given by Eqs. (2) are represented in the form

$$\begin{aligned} h_z^0 &= \cos(\theta + \Sigma_{12})\cos\Sigma_{11} + R\cos(\theta + \Sigma_{22})\cos\Sigma_{21}, \\ h_x &= \sin(\theta + \Sigma_{12})\cos\Sigma_{11} + R\sin(\theta + \Sigma_{22})\cos\Sigma_{21}. \end{aligned}$$

The longitudinal field on each spin gives the energy density per unit interval of the coordinate space equal to the lattice constant

$$\begin{aligned} h_{\|} = \varepsilon &= h_z\cos\theta + h_x\sin\theta = \delta h_z^0\cos\theta + \varepsilon_0, \\ \varepsilon_0 &= \cos\Sigma_{11}\cos\Sigma_{12} + R\cos\Sigma_{21}\cos\Sigma_{22}, \end{aligned} \tag{4}$$

where δh_z^0 is the anisotropy field and ε_0 is the energy of the frustrated exchange field in the isotropic case $\delta = 0$.

The orientation of each spin is unambiguously determined by the condition of its collinearity to the total local field from neighboring spins. It is expressed mathematically in the requirement of vanishing of the field components orthogonal to the direction of the spin (in our case, the transverse component in the polarization plane of the helicoid)

$$\begin{aligned} h_\perp &= h_z\sin\theta - h_x\cos\theta = \delta h_z^0\sin\theta - \Delta_0 \equiv 0, \\ \Delta_0 &= \cos\Sigma_{11}\sin\Sigma_{12} + R\cos\Sigma_{21}\sin\Sigma_{22}. \end{aligned} \tag{5}$$

With allowance for this limitation, the magnetic energy density (4) takes the multiplicative form; i.e., the anisotropic and frustration components enter in the form of the product

$$\varepsilon = \frac{1+\delta}{1+\delta\sin^2\theta}\varepsilon_0. \quad (6)$$

The condition (5) takes the form of the nonlinear equation on series of derivatives

$$\frac{\cos\Sigma_{11}\sin\Sigma_{12} + R\cos\Sigma_{21}\sin\Sigma_{22}}{\cos\Sigma_{11}\cos\Sigma_{12} + R\cos\Sigma_{21}\cos\Sigma_{22}} = \frac{\delta\sin\theta\cos\theta}{1+\delta\sin^2\theta},$$

the solution of which can be obtained in the approximation of small anharmonicity ($\theta'' \ll 1$), where derivatives higher than the second order can be ignored,

$$\theta''\frac{\cos\theta' + 4R\cos 2\theta'}{\cos\theta' + R\cos 2\theta'} = \frac{2\delta\sin\theta\cos\theta}{1+\delta\sin^2\theta}.$$

The change of the variable $z = (\theta')^2/2$ makes it possible to integrate this autonomous differential equation in quadratures

$$I(z, z_0) = \int_{z_0}^{z}\frac{C(z)}{\epsilon_0}dz = \ln(1+\delta\sin^2\theta), \quad (7)$$

where $C(z) = \cos\sqrt{2z} + 4R\cos 2\sqrt{2z}$ and $\epsilon_0(z) = \cos\sqrt{2z} + R\cos 2\sqrt{2z}$. The variable z changes from the initial value z_0 at $\theta = 0$ to $z_{\max}$ at $\theta = \pi/2$.

Expanding the integral (7) in a Taylor series in powers of the deviation of the variable z from z_0

$$I(z, z_0) = \sum_{n=1}^{\infty} a_n \frac{(z - z_0)^n}{n!},$$

$$a_n = \left(\frac{C(z)}{\epsilon_0}\right)^{(n-1)}_{z_0},$$

retaining only the first two terms ($a_{n>2} = 0$ [20]), we obtain the explicit form of the dependence of the variable z on the orientation angle of the spin

$$\begin{aligned} z = z_0 &+ \frac{\varepsilon_0(z_0)}{3RK(z_0)(1+2\cos^2\sqrt{2z_0})} \\ &\times (C(z_0) - (C^2(z_0) - 6RK(z_0) \\ &\times (1+2\cos^2\sqrt{2z_0})\ln(1+\delta\sin^2\theta))^{1/2}), \end{aligned} \quad (8)$$

$$K(z_0) = \frac{\sin(\sqrt{2z_0})}{\sqrt{2z_0}}.$$

The number of spins in the unit interval of the angle θ (the spin density d) is determined by the angular velocity and depends on the initial condition and the angle θ:

$$d = (\theta')^{-1} = (2z(z_0, \theta))^{-1/2}. \quad (9)$$

Substituting the expression for the angular velocity into the energy density (6) and integrating over the periodicity interval of the function $\sin^2\theta$, we obtain the average energy per spin

$$E_S(z_0) = \frac{(1+\delta)\int_0^{\pi/2}\frac{\varepsilon_0(z)}{1+\delta\sin^2\theta}\frac{d\theta}{\sqrt{2z(\theta, z_0)}}}{\int_0^{\pi/2}\frac{d\theta}{\sqrt{2z(\theta, z_0)}}}. \quad (10)$$

The ground state of solutions obtained is determined by the extremum of the energy (10) (in our case, the maximum, since the fields and the energy density are given in units of ferromagnetic exchange $J_1 < 0$). The value $z_0 = z_{\min}$ corresponding to this extremum specifies the ground state of the soliton lattice for each set of the parameters δ and R. After the substitution of this value into Eq. (9), we obtain the dependence of the angular velocity on the angle in the ground state. We note that the explicit dependence of the angle on the spatial coordinate is not required for the calculation of the energy of the soliton lattice because the initial problem is translationally invariant.

The average energy of the ground state of the soliton lattice (10) depends nonlinearly on the anisotropy parameter δ (Fig. 1). The first-order phase transition in this parameter to the ferromagnetic state (F) (at $|R| < 1/2$) or to the state with the alternation of pairs of spins directed along and opposite to the z axis (up–up–down–down (UUDD) phase) (at $|R| > 1/2$) [11–13] occurs at the coincidence of the energy of the soliton lattice with the energy of the collinear phase:

$$E_F = (1+\delta)(1+R), \quad |R| < 1/2,$$

$$E_{UUDD} = -(1+\delta)R, \quad |R| > 1/2.$$

The difference between the minimum ($z_{\min}$) and maximum ($z_{\max}$) values of the variable z increases monotonically with δ and reaches the maximum at the triple point ($R = -1/2$, $\delta \approx 1.34$). Figure 2 shows the changes in the energy density ε, the spin density d, and the parameter z as functions of the orientation angle of spins at the triple point.

The limits of the variation of the variable z at other points of interfaces (solid lines), as well as its value for the helicoid with the constant step ($\delta = 0$) at the same R values (dotted line) for comparison, are shown in the phase diagram of the ground state of the model (1) (Fig. 3). Such helicoid with the polarization plane orthogonal to the anisotropy axis also satisfies the collinearity condition. However, its normalized energy equal to the energy in the absence of the anisotropy,

$$E_S(\delta = 0) = -R - \frac{1}{8R}, \quad (11)$$

is always less than the monotonically increasing energy of the soliton lattice (see Fig. 1). Thus, at any easy-axis anisotropy, the soliton lattice with the polar-

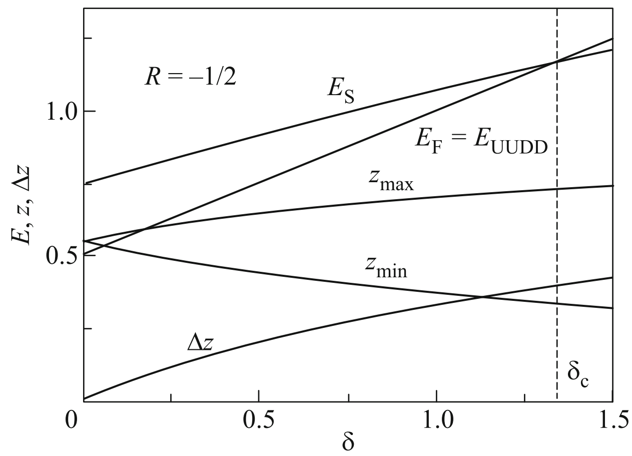

Fig. 1. Average energy of the soliton lattice E_S, the limiting values of the variable z (the square of the angular velocity), and the interval of its variation with the anisotropy at $R = -1/2$. The change in the energy of collinear phases at this frustration parameter is also shown.

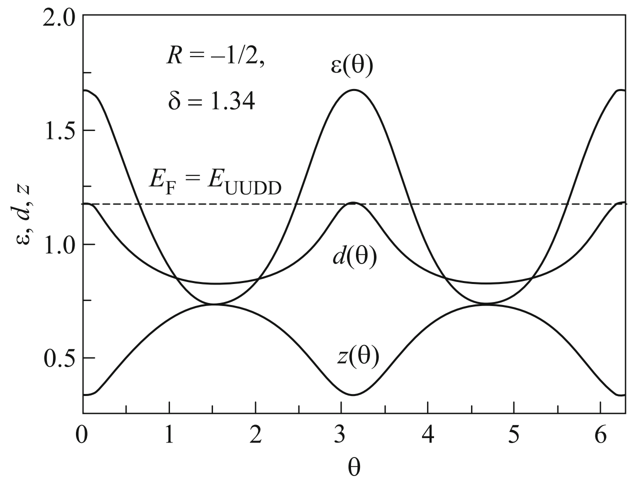

Fig. 2. Normalized energy density of the helicoid with the variable step ε(θ) (6), the number of spins per unit angle interval (the spin density) $d(\theta)$ (9), and the variable z (8) versus the angle θ at the triple point of the phase diagram.

ization plane containing the anisotropy axis is energetically more favorable than that of a uniform planar helix. The condition of the collinearity of spins to local fields limits also the formation of the uniform conical helicoid: either the external magnetic field or the exchange field from spins of the second magnetic subsystem is additionally necessary for its existence.

The phase diagram of the ground state of the quantum model (1) with the easy-axis anisotropy $\delta_1 = \delta_2 = \delta > 0$ contains three phases: ferromagnetic (F), antiferromagnetic with pairs of spins oriented along and opposite to the axis z (UUDD phase), and the intermediate phase with the magnetization, which is a continuous function of the parameters of the model [11–13]. The model (1) with classical spins is considered in [18] for the case $\delta_1 > \delta_2 = 0$ near the Lifshitz point $|R| = 1/4$, and the integral of the magnetic energy density was minimized at $\delta_1 = 0$. In our approach in the absence of the anisotropy of the exchange with next-nearest neighbors, the collinearity equation is no longer autonomous and its solution can be found in the form of the correction over the argument of the function $z(\delta_1 \sin\theta)$ to the solution of the autonomous equation.

For comparison, Fig. 4 shows interfaces between soliton and ferromagnetic phases for the cases (*1*) $\delta_1 = \delta_2 = \delta$ and (*2*) $\delta_1 > \delta_2 = 0$ in the corresponding region of the phase space. The quadratic dependence of the interface $\delta_{1c} \propto R^2$ coinciding with the result [18] (curve *3*) remains only in the nearest neighborhood of the Lifshitz point. With an increase in $|R|$, this dependence becomes linear, which can be easily explained. With an increase in the frustration, the angle between the nearest spins tends to $\pi/2$; i.e., the incommensurate structure with the local spin orientation of the "cross" type is formed. At this energy, such structure (11) has the asymptotic behavior $\varepsilon(|R| \to \infty) = -R$, which gives the asymptotic interface $\delta_{1c} = -2R - 1$ in the comparison with the energy of the ferromagnetic phase. At the same time, for the case with the anisotropy in both exchanges, such asymptotic behavior is $\delta_c = (1 + R)^{-1}$. At the anisotropy $\delta_1 > \delta_2 = 0$ and $|R| \approx 0.35$, the maximum velocity

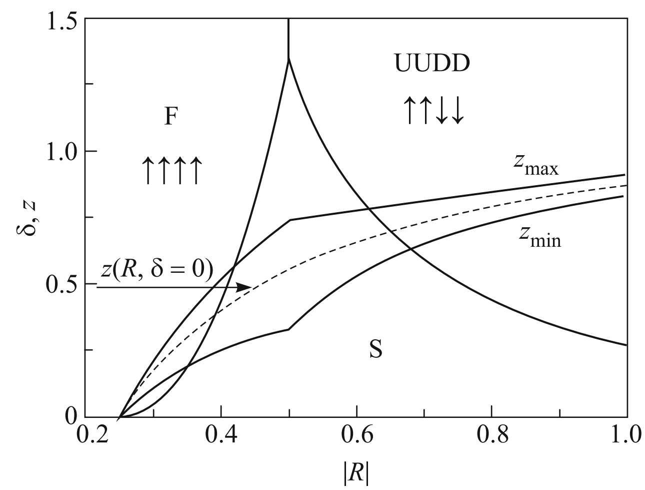

Fig. 3. Phase diagram of the classical easy-axis frustrated ferromagnet. Limits of variation of the variable $z(\theta)$ at interfaces between the soliton (S), ferromagnetic (F), and UUDD phases are shown in comparison with the dependence $z(|R|)$ for the uniform planar helicoid. At $|R| \to \infty$, the interface between UUDD and soliton phases tends to the $|R|$ axis.

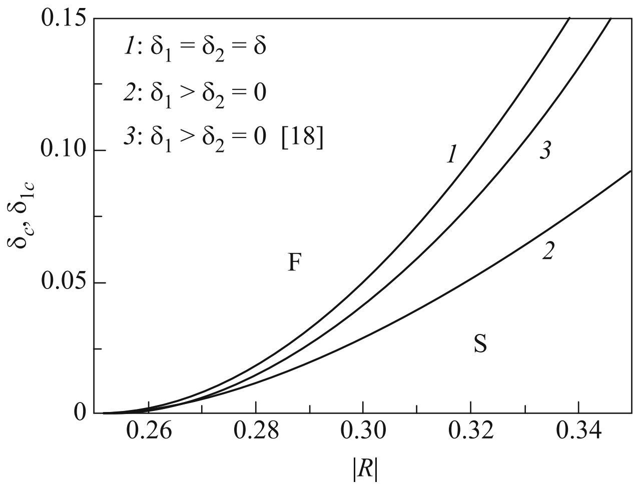

Fig. 4. Interface between the ferromagnetic and soliton phases of the classical easy-axis frustrated ferromagnet near the point $|R| = 1/4$ for two cases of the anisotropy of the model (1). Dependence *3* is taken from [18].

(the angle between neighboring spins at $\theta \approx \pi/2$) exceeds $\pi/4$, and that for next-nearest neighbors exceeds $\pi/2$. At large frustration parameters, the replacement of trigonometric functions of the velocity in the energy density and the variational Euler equation will give a considerable systematic error. In the equation on the collinearity of spins and fields, we substituted the argument of trigonometric functions of the second derivative of the angle θ, which even at the maximum value at the triple point of the phase diagram (see Fig. 3) does not exceed 0.45.

The comparison of two different cases of the exchange anisotropy of the model (1) shows that the statement about the insignificant effect of the anisotropy of the exchange with next-nearest neighbors we made in [11] (and in a series of works of other authors) is wrong. The absence of such anisotropy qualitatively changes the phase diagram, since the energy of the UUDD phase always becomes higher than the energy of the soliton lattice. The absence of the UUDD phase on the phase diagram of the classical model (1) at $\delta_2 = 0$ indicates the possible changes also on the quantum phase diagram, where this phase is present at $\delta_2 > 0$ [11–13].

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Translated by L. Mosina