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Continual approach at T=0 in the mean field theory of incommensurate magnetic states in the frustrated Heisenberg ferromagnet with an easy axis anisotropy

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ABSTRACT

The algorithm of approximate solution was developed for the differential equation describing the anharmonical change of the spin orientation angle in the model of ferromagnet with the exchange competition between nearest and next nearest magnetic neighbors and the easy axis exchange anisotropy. The equation was obtained from the collinearity constraint on the discrete lattice. In the low anharmonicity approximation the equation is resulted to an autonomous form and is integrated in quadratures. The obvious dependence of the angle velocity and second derivative of angle from angle and initial condition was derived by expanding the first integral of the equation in the Taylor series in vicinity of initial condition. The ground state of the soliton solutions was calculated by a numerical minimization of the energy integral. The evaluation of the used approximation was made for a triple point of the phase diagram.

1. Introduction

The theoretical description of incommensurate magnetic structures (IMS) in antiferromagnetic dielectrics in the framework of Landau phenomenological theory of the phase transition was elaborated by Dzyaloshinskii [1]. For helimagnet with the Dzialoshinskii–Moria antisymmetrical exchange leading to a Lifshitz invariant in a free energy expansion (relativistic mechanism of forming IMS) the energy minimization for the solutions within the anisotropic plane is reduced to the solution of static sine-Gordon equation. The equation has the anharmonic solutions in the form of elliptical integrals describing the inhomogeneous helical structure with the step changing when moving along the helix vector – the so-called soliton lattice [2]. The inhomogeneous magnetoelectric interaction also leads to the Lifshitz invariant and, hence, to the sine-Gordon equation with the same solutions as shown for the thorough investigated multiferroic $BiFeO_3$ [3,4]. For helimagnets with competing exchange interactions between the nearest and further magnetic neighbors (the exchange mechanism of incommensurability) it is necessary to take into consideration the second derivatives (and higher ones in the general case) of an order parameter. So the energy minimization cannot be reduced to an analytically integrable differential equation.

The aim of the present work is to develop the algorithm of approximate solution for the differential equation describing the anharmonical change of the spin orientation angle in the model of easy axis ferromagnet with the exchange competition between the nearest and next nearest magnetic neighbors. We consider the magnetic structure with the spin orientation within the anisotropy plane (the flat anharmonic helix) and depending on the one coordinate. As the initial equation the constraint of the spin collinearity to the total exchange field from the neighboring spins is used. The application of such an approach for the frustrated ferrimagnet on the discrete lattice allowed us to describe the flat and conical IMS and to obtain the phase diagrams [5,6]. The second order differential equation is obtained from the general one containing all the derivatives of the spin orientation angle in the approximation of slow variation of the helical step (the low helix anharmonicity). To analytically solve the equation with regard to the first derivative of the angle (the angle velocity) the first integral of the differential equation (the solution in quadratures) is expanded to the Taylor series over the square of the velocity up to the second power. All anharmonic solutions are parametrized by the value of velocity in the expansion point, in our case at the spin orientation along the easy axis. The ground state is chosen through the numerical minimization of the energy of spins on the quarter of period.

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2. Model and approach

The Hamiltonian of the model with the ferromagnetic and antiferromagnetic exchanges between nearest and next nearest neighbors and the easy axis exchange anisotropy (XXZ-model) has a form

$$H = J_1 \sum_i (\mathbf{S}_i\mathbf{S}_{i+1} + \delta S_i^z S_{i+1}^z) + J_2 \sum_i (\mathbf{S}_i\mathbf{S}_{i+2} + \delta S_i^z S_{i+2}^z), \quad J_1 < 0, \quad J_2 > 0, \quad \delta > 0, \tag{1}$$

where $\mathbf{S}_i$ is a unit vector on the site i. In this model the same relative anisotropy of the exchanges between the nearest and next nearest exchanges is considered. This variant of anisotropy allows us to reduce the number of model parameters and simply separate an effect of frustration and anisotropy on the IMS energy. The case of generalization on different anisotropy is easy realized and does not essentially change the result. The orientation of the spin S_i in the plane with the easy axis z is determined by the total exchange field from neighbor spins $S_{i\pm1}$ and $S_{i\pm2}$. At T=0 all spins have the equal length equal to saturation one and the field normalized on the exchange J_1 has the components

$$h_z = (1+\delta)h_z^0, \quad h_z^0 = \tfrac{1}{2}(\cos\theta_{i+1} + \cos\theta_{i-1} + R(\cos\theta_{i+2} + \cos\theta_{i-2})), \quad h_x = \tfrac{1}{2}(\sin\theta_{i+1} + \sin\theta_{i-1} + R(\sin\theta_{i+2} + \sin\theta_{i-2})), \tag{2}$$

where $h^0{}_z$ is the z-component of exchange field without anisotropy, θ is a polar angle and $R = J_2/J_1 < 0$ is a frustration parameter. The transition to the continual description is carried out by the Taylor series expansion of the neighbor spins angles for the each site i

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

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

$$\Sigma_{11} = \sum_{n=1}^{\infty} \frac{\theta^{(2n-1)}}{(2n-1)!}, \quad \Sigma_{22} = \sum_{n=1}^{\infty} \frac{2^{2n}\theta^{(2n)}}{(2n)!}, \quad \Sigma_{12} = \sum_{n=1}^{\infty} \frac{\theta^{(2n)}}{(2n)!}, \quad \Sigma_{21} = \sum_{n=1}^{\infty} \frac{2^{2n-1}\theta^{(2n-1)}}{(2n-1)!}.$$

After substituting (3) the components (2) take the forms

$$h_z^0 = \cos(\theta + \Sigma_{12})\cos\Sigma_{11} + R\cos(\theta + \Sigma_{22})\cos\Sigma_{21}, \quad h_x = \sin(\theta + \Sigma_{12})\cos\Sigma_{11} + R\sin(\theta + \Sigma_{22})\cos\Sigma_{21}. \tag{4}$$

The longitudinal field on the spin is equal to an energy density on the single interval in coordinate space (on one spin)

$$h_{\parallel} = \epsilon = h_z\cos\theta + h_x\sin\theta = \delta h_z^0\cos\theta + \epsilon_0, \quad \epsilon_0 = \cos\Sigma_{11}\cos\Sigma_{12} + R\cos\Sigma_{21}\cos\Sigma_{22},$$

where ϵ_0 is an energy in the isotropic case $\delta = 0$. An orientation of each spin is uniquely determined by the collinearity condition of spins and local fields from the neighbor spins [7]. This constraint allows to avoid the nonphysical states and to determine all allowable states including the excited ones. So, the transverse field on the spin must be equal to zero

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

Taking into account the collinearity constraint (5) the magnetic energy density takes a multiplicative form – the anisotropic and frustration contributions are contained as product terms

$$\epsilon = \frac{1+\delta}{1+\delta\sin^2\theta}\cdot\epsilon_0. \tag{6}$$

Rewriting the general Eq. (5) in the following form:

$$\frac{\cos\Sigma_{11}\sin\Sigma_{12} + R\cos\Sigma_{21}\sin\Sigma_{22}}{\cos\Sigma_{11}\cos\Sigma_{12} + R\cos\Sigma_{21}\cos\Sigma_{22}} = \frac{\delta\sin\theta\cos\theta}{1+\delta\sin^2\theta}, \tag{7}$$

one can make a general conclusion that anharmonicity in the change of angle θ (the derivatives of the second order and higher) appeared at $\delta > 0$, takes a maximum value at intermediate angles $\theta \approx (2n+1)\pi/4$ and vanishes at $\theta = n\pi/2$.

Further solution of Eq. (7) will be made in the linear anharmonicity approximation ($\theta'' \ll 1$), neglecting the derivatives which are higher than second order. In this approach Eq. (7) takes an autonomous form

$$\theta''\cdot\frac{\cos\theta' + 4R\cos2\theta'}{\cos\theta' + R\cos2\theta'} = \frac{2\delta\sin\theta\cos\theta}{1+\delta\sin^2\theta}, \tag{8}$$

and at the substitution $z = (\theta')^2/2$ is integrated in quadratures

$$I(z, z_0) = \int_{z_0}^{z} \frac{C(z)}{\epsilon_0} dz = \ln(1+\delta\sin^2\theta), \tag{9}$$

where $C(z) = \cos\sqrt{2z} + 4R\cos2\sqrt{2z}$, $\epsilon_0(z) = \cos\sqrt{2z} + R\cos2\sqrt{2z}$. The variable z changes in the range $\{z_0, z_{max}\}$ at $\theta \in \{0, \pi/2\}$. Expanding the integral in the Taylor series in vicinity of z_0 and taking into account that $I(z = z_0) = 0$ we obtain the series

$$I(z, z_0) = \sum_{n=1}^{\infty} a_n\cdot\frac{(z-z_0)^n}{n!}, \quad a_n = \left(\frac{C(z)}{\epsilon_0}\right)_{z_0}^{(n-1)}. \tag{10}$$

At the low anharmonicity keeping first two nonzero terms of series (10) (the quadratic approximation) we obtain the obvious dependence of the angle velocity from angle and initial condition z_0:

$$z = z_0 + \frac{\epsilon_0(z_0)}{3R\cdot K(z_0)(1+2\cos^2\sqrt{2z_0})} \cdot (C(z_0) - (C^2(z_0) - 6R\cdot K(z_0) \cdot (1+2\cos^2\sqrt{2z_0})\ln(1+\delta\sin^2\theta))^{1/2}), \tag{11}$$

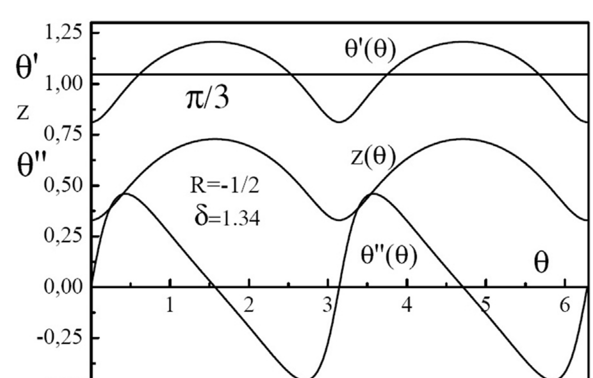

Fig. 1. The angle dependences of the variable z, the step of IMS θ' and the second derivative θ''. The line $\pi/3$ corresponds to the constant IMS step at $R = -1/2$ and $\delta = 0$.

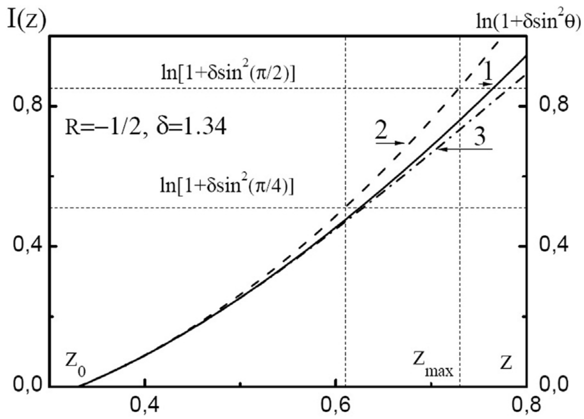

Fig. 2. The result of numerical integration of the first integral (9) (solid line 1) and quadratic (dash line 2) and cubic (dash-dot line 3) approximations. The horizontal dash lines show the right part of Eq. (9) at $\theta = \pi/4$ and $\pi/2$.

where

$$K(z_0) = \frac{\sin(\sqrt{2z_0})}{\sqrt{2z_0}}. \quad (12)$$

As the energy (6) and the angle velocity (11) depend on $\sin^2\theta$ the energy over the quarter of period divided by the corresponding length is equal to the average energy of one spin:

$$E_S(z_0) = \frac{(1+\delta)\int_0^{\pi/2} \frac{\epsilon_0(z)}{1+\delta\sin^2\theta} \frac{d\theta}{\sqrt{2z(\theta, z_0)}}}{\int_0^{\pi/2} \frac{d\theta}{\sqrt{2z(\theta, z_0)}}}.$$

The ground state of the solutions is determined by an extreme of the function (the maximum in our case, because fields and energy density are normalized on the $J_1 < 0$). The corresponding initial condition $z_0 = z_{extr}$ parametrizes the ground state solution for each set of the parameters δ and R and after substituting into Eq. (11) determine the functional dependence of z on the angle θ in the ground state (Fig. 1). Note that to determine the average energy of the spins and hence to compare it with the energy of the collinear states the dependence of θ on the coordinate r is not required.

3. Discussion

We discuss the properties of the solutions corresponding to the soliton-like ground state. The solutions with increasing spiral step upon changing the angle between the spin and easy axis θ from zero to $\pi/2$ ($\theta'' > 0$) exist when the numerator of fraction in the left part of (8) is positive-defined. Developing the cosines in the series up to second power of θ' we obtain the condition imposed on the initial spin velocity

$$z_0 \geq z_{min} = \frac{1+4R}{1+16R} \geq 0. \quad (13)$$

The solutions can be obtained when the general classical condition $|R| \geq 1/4$ is fulfilled [8]. It is impossible for the IMS wave vector to tend to zero at the phase transition from the incommensurate to commensurate state, which also follows from the phenomenological analysis based on the Landau theory [2]. It means that the transition on the model parameters δ and R is accompanied by a step-like change of the magnetic structure vector and hence is the first order phase transition.

The application of the first integral expansion in series over the powers of $z - z_0$ (10) impose, in general, a limitation on the anisotropy parameter value δ inducing the anharmonicity. The range of the z variation from z_{extr} to z_{max} is increased with increasing δ and takes a maximal value on the phase boundary with collinear phases. The difference $z_{max} - z_{extr}$ takes the maximum value equal to 0.4 in the triple point $R = 1/2$, $\delta \approx 1.34$ where the energy of the soliton phase is equal to the energies of ferromagnetic and “up-up-down-down” phases [9]. To assess the application of the quadratic approximation at the expansion of the first integral (9) one makes a numerical integration in the triple point and compares the result with the quadratic and cubic decomposition (10) (Fig. 2). The coefficients a_1 and a_2 are positive. The third coefficient a_3 is negative and together with the next terms of expansion forms an alternate series which provides a fast expansion convergence to the numerical integration result even for the limit difference in the triple point of the phase diagram. The autonomous differential equation (8) was obtained in the linear approximation on the second derivative θ''. The limit value of the second derivative in the triple point is equal to 0.45 (Fig. 1) which allows one to argue that the used approach provides at least a qualitatively correct description of the soliton ground states in the whole range of their existence. Note, that the present approach does not impose a limitation on the absolute value of the angle change velocity (the helix step) and it is applicable both for long-period IMS and for the structures with a comparatively short period.

In summary, the continual approach based on the collinearity of the spins and corresponding total fields allows one to solve in quadratures the differential equation on the spiral step in the anisotropic plane. The decomposition of the first integral in Taylor series shows the fast convergence to the result of numerical integration and leads to the angle dependences of the solution parameters in a simple analytical form. The phase transition over the frustration and anisotropy parameters between the anharmonical spiral (soliton) phase and collinear ferromagnetic and “up–up–down–down” phases is a first order one.

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