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Ground State of an Antiferromagnet with Uniform Antisymmetric Exchange in a Magnetic Field

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A system of two nonlinear differential equations for sublattice angles is proposed to describe the spin orientation distribution in a planar antiferromagnet with uniform antisymmetric exchange in a magnetic field. This system involves the initial symmetry of the problem and is reduced to a single delay differential equation. The solutions of this system are parameterized by the initial condition imposed on the angle of one sublattice at the hyperbolic singular point of the phase space. The numerical analysis of the stability boundary of soliton solutions demonstrates that the transition to the commensurate phase takes place outside the region where the stochastic solutions appear and is accompanied by the magnetization jump $\Delta m \sim 10^{-1}m$.

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The field dependence of the magnetization is one of the key criteria of the correct determination of the magnetic structure type. The critical magnetic field at which this dependence changes qualitatively is determined by the formation mechanisms of this structure and is the main source of information on them. The incommensurate magnetic structure (IMS) of an antiferromagnet with antisymmetric exchange

$$H = \sum_{r,a}[J\mathbf{S}_r\mathbf{S}_{r+a} + \mathbf{D}[\mathbf{S}_r \times \mathbf{S}_{r+a}] - \mathbf{H}_o\mathbf{S}_r] \quad (1)$$

in the vicinity of the field transition to the commensurate magnetic phase has the form of a soliton lattice where magnetic moments change their spatial orientation with a variable rate [1, 2]. Even in the simplest 2D case, its mathematical description is rather cumbersome. Although methods for solving the nonlinear differential equations of spin dynamics have recently been successfully developed [3], these equations can be analytically solved only under some significant simplifications of the initial problem, which narrow the applicability of this approach. For example, being used in the Euler variation procedure, the Dzyaloshinskii approximation conventionally used in the phenomenological description with the energy functional containing the Lifshitz invariant in the form

$$I_L \sim b\rho^2\frac{\partial\varphi}{\partial x}, \quad \rho \text{ is const}, \quad (2)$$

where ρ is the amplitude of the order parameter and φ is the angle of its orientation on the plane, leads to the mathematical pendulum equation independent of the initial mechanism of incommensurability—the parameter b (antisymmetric exchange D in Eq. (1)),

$$\frac{\partial^2\varphi}{\partial x^2} + c\frac{H_0^2}{J^2S^2}\sin 2\varphi = 0. \quad (3)$$

As a result, the IMS energy is calculated on the phase space trajectories (Fig. 1) corresponding to the zeroth approximation of the problem, which is the system without antisymmetric exchange. Obviously, this approach can be considered appropriate only when the latter is small.

Another important restriction of approximation (1) is the constancy of the order parameter magnitude and manifests itself in the estimation of the solution stability near the transition to the commensurate phase [2, 4, 5]. The incommensurate solution loses stability before the energy minimum approaches a sin-

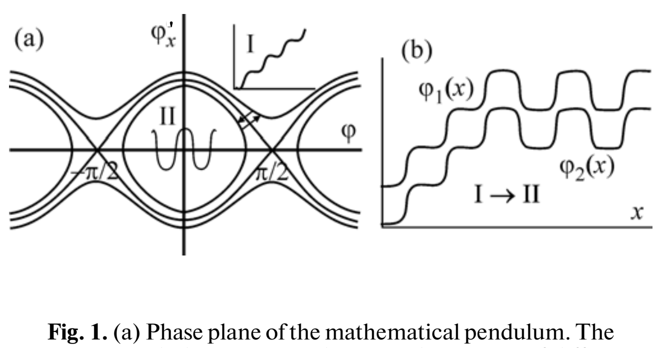

Fig. 1. (a) Phase plane of the mathematical pendulum. The arrows mark the transitions between the regions of different-type solutions. (b) The transition between the regions for system of equations (6).

gle-soliton solution (the separatrix in Fig. 1). The magnitude of the order parameter, which is the length of the antiferromagnetism vector, varies with the angle between the sublattices even at $T = 0$, and this is most pronounced in the soliton phase in the regions of the fast reorientation of the moments, i.e., in the domain walls.

The description of the states of the classical two-dimensional spin Hamiltonian (an analog of the two-parameter model in the phenomenological description) reduces in the continual approximation to the solution of the differential equation of the one-dimensional mathematical pendulum (the sine-Gordon equation) by only changing the initial trigonometric functions to their variables and discarding the derivatives with respect to the angle between the antiferromagnetism vector and the sublattice moment direction [6]. The subsequent calculation of the energy and magnetization of the incommensurate magnetic structure on the unexcited trajectories of the mathematical pendulum provides the same fundamental result as approximation (2) of the phenomenological approach, i.e., the second-order phase transition to the commensurate phase.

The most serious consequence of the replacement of the initial discrete problem with Hamiltonian (1) by the continual approximation can be the complete loss of the stochastic solutions in the vicinity of the singular points and trajectories of the phase space. In this approximation, the stochastic solutions are absent in the one-component systems [7]. An example is exactly integrable equation (3). Meanwhile, the discrete anisotropic chain of spins near the separatrix has the domain of stochastic solutions as has been shown for the ferromagnets and antiferromagnets with dipole interaction [8] and for a ferromagnet with antisymmetric exchange [2]. Approaching the transition point to the commensurate phase, the trajectory of the soliton solution with the minimum energy either passes from region I to the region of stochastic solutions near the separatrix or has energy coinciding with that of the canted antiferromagnetic structure in the region of stable closed solutions. In the latter case, the transition will occur from a finite value of the soliton lattice period and will be accompanied by the jump of the magnetization. The implementation of the above transitions is controlled by the width of the stochastic layer around the separatrix (the anisotropy parameter value) [9]. The energies of the commensurate phase in a ferromagnet and an antiferromagnet are the linear and quadratic functions of the applied magnetic field, respectively. For the S ions, the relation $D \ll J$ is usually valid, the destruction field of the incommensurate magnetic structure is low; therefore, the energy of the commensurate phase of the ferromagnet decreases to the IMS energy much faster than it occurs in the antiferromagnet. The critical field of the antiferromagnet is two or three orders of magnitude higher than that of the ferromagnet at the same exchange magnitudes. Hence, the probability of the first order transition to the commensurate phase via the stochastic destruction of the incommensurate magnetic structure is higher.

To study the IMS behavior in the magnetic field, we consider the classical Hamiltonian of the model [6] without the above simplifications:

$$\begin{aligned} H = \sum_n [JS^2\cos(\varphi_{n+1} - \varphi_n) \\ + DS^2\sin(\varphi_{n+1} - \varphi_n) - H_o S\cos\varphi_n]. \end{aligned} \tag{4}$$

The variation of the energy with respect to the variables φ_n leads to the finite-difference equations of the discrete problem,

$$\begin{aligned} &\sin(\varphi_n - \varphi_{n+1} + \arctan d) \\ &+ \sin(\varphi_n - \varphi_{n-1} - \arctan d) - \frac{h}{2\sqrt{1+d^2}}\sin\varphi_n \\ &= 2\sin\left(\varphi_n - \frac{\varphi_{n+1} + \varphi_{n-1}}{2}\right)\cos\left(\frac{\varphi_{n+1} - \varphi_{n-1}}{2} - \arctan d\right) \\ &- \frac{h}{2\sqrt{1+d^2}}\sin\varphi_n = 0, \end{aligned} \tag{5}$$

where $d = D/J$ and $h = H_0/JS$. The continual transition to the smooth functions of the angles of two antiferromagnetic sublattices φ_1 and φ_2 including the terms up to the second-order derivatives,

$$\varphi_{1,2}(x \pm 1) = \varphi_{1,2}(x) \pm \frac{\partial\varphi_{1,2}}{\partial x} + \frac{1}{2}\frac{\partial^2\varphi_{1,2}}{\partial x^2},$$

yields the system of two second-order nonlinear differential equations

$$\begin{aligned} &\sin\left(\varphi_1 - \varphi_2 - \frac{1}{2}\frac{\partial^2\varphi_2}{\partial x^2}\right)\cos\left(\frac{\partial\varphi_2}{\partial x} - \arctan d\right) \\ &- \frac{h}{2\sqrt{1+d^2}}\sin\varphi_1 = 0, \\ &\sin\left(\varphi_2 - \varphi_1 - \frac{1}{2}\frac{\partial^2\varphi_1}{\partial x^2}\right)\cos\left(\frac{\partial\varphi_1}{\partial x} - \arctan d\right) \\ &- \frac{h}{2\sqrt{1+d^2}}\sin\varphi_2 = 0. \end{aligned} \tag{6}$$

In contrast to the one-dimensional, one-component dynamical system, the system of two coupled nonlinear pendulums is integrable only with the special choice of the parameters ensuring the separation

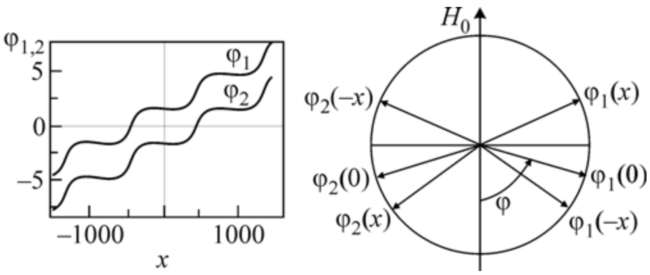

Fig. 2. Symmetry of soliton solutions of type I.

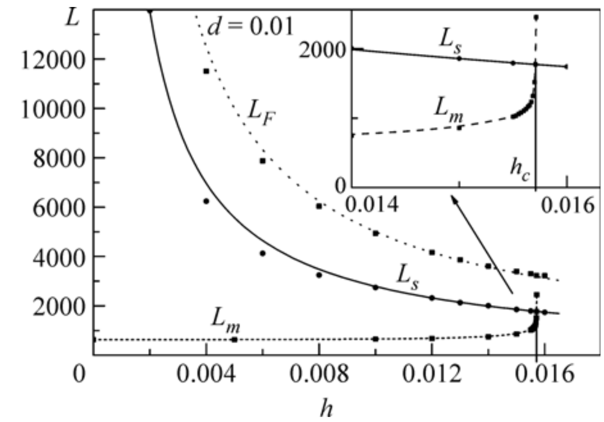

Fig. 3. Field dependences of the ultimate stable periods L_F and L_S of finite-difference equation (5) and the system of differential equations (6), respectively, as well as the minimum-energy period L_m of the soliton lattice. The solid and dashed lines are Eqs. (9) and (11), respectively.

of the variables [10]. Therefore, in the general case, system (6) retains its stochastic properties in the vicinity of the disappearance of the IMS. This system, as well as pendulum equation (3), has two types of closed periodic solutions separated by the separatrix on the phase plane. The first-type soliton solutions (I) with a lower energy at $h < h_c$ are symmetric with respect to the second-order axis passing through the origin $x = 0$ chosen from the condition $\varphi_2(0) = -\varphi_1(0)$ (the hyperbolic singular point $\varphi = \pi/2$ in Fig. 1). The axis is orthogonal to the plane of the solutions $\varphi_{1,2}(x)$, is parallel to the applied magnetic field (see Fig. 2), and presents the symmetry of initial system (6), which is transformed into itself under the turn $\varphi_1 \longleftrightarrow -\varphi_2$, $x \longrightarrow -x$. The symmetry of the equations and their solutions follows from the initial symmetry of the problem. The antisymmetric exchange implies the absence of the inversion center between the magnetic ions in the symmetry elements of the crystal (and, hence, the presence of the odd-order derivatives in the equations) and allows for the existence of the second-order axis or the mirror plane between them [11]. The sine-Gordon equation does not satisfy this symmetry.

This choice of the origin allows us to parameterize the solution by a single initial value of $\varphi_1(0)$. Taking into account that $\varphi_1''(0) = \varphi_2''(0) = 0$ at this point, the initial conditions for the velocities are obtained from Eq. (6) in the form

$$\varphi_1(0)' = \arctan d \pm \arccos\left(\frac{h}{2\sqrt{1+d^2}\cos\varphi_1(0)}\right), \quad (7)$$
$$\varphi_2(0)' = \varphi_1(0)'.$$

The lower-energy trajectories are closer to the separatrix; i.e., the initial velocities are specified by the minus sign in Eq. (7). The symmetry of the solutions of system (6) with respect to the chosen origin makes it possible to reduce the system to a single delay differential equation in the variable $y(x)$, which, depending on the initial condition, describes the spatial orientation distribution of every sublattice,

$$\sin(y(x) + y(-x) + y''(-x)/2)\cos(y'(-x) - \arctan d)$$
$$-\frac{h}{2\sqrt{1+d^2}}\sin y(x) = 0, \quad (8)$$
$$y(x) \equiv \varphi_1(x), \text{ if } y(0) = \pi/2 - \delta,$$
$$y(x) \equiv \varphi_2(x), \text{ if } y(0) = -\pi/2 + \delta.$$

The solutions near the separatrix are very sensitive to the variation of the initial conditions under which the solution of system (6) is sought. The limited accuracy of the numerical calculations results in small fluctuations of the trajectory, which have the same effect. As a result, the period of the soliton solution in the stochastic phase is changed and the transitions from region I to region II and back appear over large ranges of the solution search ($x > 10^5$ lattice constants) (see Fig. 1). Although such a criterion of the appearance of stochasticity is conditional, it allows for the simple and clear representation of the qualitative rearrangement of the state. We estimate the solution stability boundary with respect to these transitions. The soliton lattice period L_s (Fig. 3) at which the stability is lost and the transitions between the regions with different types of the soliton solution begin is a decreasing function of the reduced magnetic field and is well approximated by the dependence

$$L_s \approx \alpha/h. \quad (9)$$

The soliton lattice period L_m corresponding to the minimum-energy trajectory varies slightly up to the critical region where it increases sharply (see Fig. 3). The point of the intersection of these two curves bounds the range of the validity of the numerical solutions of system (6). The IMS energy given by Eq. (4)

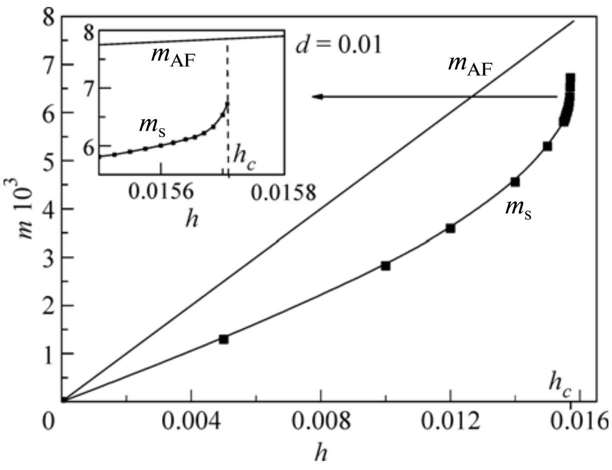

Fig. 4. Field dependences of magnetizations m_s and m_{AF} of the IMS and antiferromagnet, respectively. The inset shows the critical region.

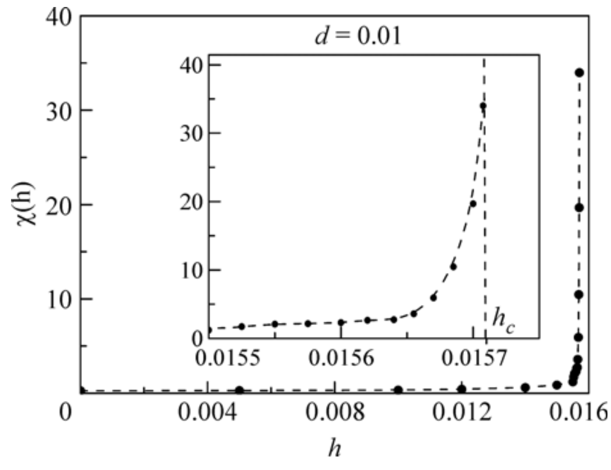

Fig. 5. Field dependence of the susceptibility. The inset shows the critical region.

calculated at the period L_m corresponding to the field coincides with the energy of the canted antiferromagnetic structure (the commensurate phase) at the stability boundary, and this allows us to conclude that the critical period of the soliton lattice is finite. In this case,

$$h_c = \frac{\pi}{2}d, \tag{10}$$

which differs from the calculation results on the pendulum trajectories [6]. This difference appears because the uniform antisymmetric exchange, in contrast to the sign-alternating exchange [11, 12], does not result in the renormalization of the antiferromagnetic exchange in the commensurate phase. The adequate asymptotic expression for the uniform solution is obtained from system (6) by assuming the derivatives to be zero.

The IMS magnetization calculated on the minimum-energy trajectories in the limit $h \longrightarrow h_c$ tends to a value lower than the antiferromagnet magnetization in the field h_c; the transition to the commensurate phase is accompanied by the magnetization jump (see Fig. 4). Accordingly, the susceptibility increases sharply near the transition point but remains finite (see Fig. 5). Thus, the field transition to the commensurate phase takes place up to the stochastic destruction of the incommensurate magnetic structure and has features of the first-order phase transition. An increase in the antisymmetric exchange up to $d = 0.1$ leads to the relevant quantitative variation of the periods and the critical field without a qualitative change in the result. The jump of the relative magnetization remains the same, $\Delta m/m \sim 10^{-1}$.

To conclude, we note the principal difference between initial problem (1) and the case with dipole interaction [8]. The change of variables $\mathbf{r} \longrightarrow -\mathbf{r}$ (the permutation of the subscripts of the spins in Eq. (1)) changes the Hamiltonian. This is the feature of the uniform antisymmetric exchange. This change of variables is equivalent to $t \longrightarrow -t$ in the dynamical systems. Therefore, finite-difference equations (5) and the system of differential equations (6) belong to the class of irreversible non-Hamiltonian systems. Hence, they can have some special trajectories qualitatively differing from the stochastic solutions considered above and the solutions for the case with the dipole interaction [8]. These trajectories are near the stability boundary of the periodic solutions of finite-difference equations (5). An analysis of the latter equations is beyond the scope of this paper. We only note that this boundary

$$L_F \approx \beta/h \tag{11}$$

is above the stability boundary of system (6) and the values of the minimum-energy periods (see Fig. 3), and these solutions including the periods close to the boundary values L_F have energy higher than the energies of the ground state of the IMS and the commensurate phase.

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