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Interaction of two spin subsystems with different wavevectors

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abstract

The possibility of the transition of a spin system from an incommensurable to a commensurable phase via a phase with different wavevectors of individual subsystems is shown in the mean-field approximation.

1. Introduction

A number of works on the study of the properties of CuB_2O_4 copper metaborate in strong magnetic fields at temperatures below 10 K have attracted attention to the subject stated in the title. In this temperature region, in the absence of a field, the magnetic structure of the crystal represents a helicoid along the tetragonal axis [1]. Further neutron diffraction study [2,3] and magnetic resonance measurements [4] showed a transition from a phase incommensurable with the crystal lattice to a phase whose magnetic structure reveals the step occurrence of both a commensurate wave and an incommensurate wave with a shorter period, with increase in the magnetic field intensity. The transition to the completely commensurate structure occurs upon further increasing the external field. Inelastic neutron scattering experiments [3] showed that the commensurate wave in the intermediate phase discovered is formed by spins of the copper ions occupying the 2b positions in an elementary cell of the crystal, whereas the incommensurate wave is formed by spins of the copper ions occupying the 4d positions. Therefore, the latter phase may be named “semi-incommensurate”.

The analysis reported in [5] demonstrated the possibility of a phenomenological description of the new phase found in the magnetic system of the copper metaborate. In the present work, the possibility of the coexistence of two magnetic subsystems with different wavevectors is considered in the mean-field approximation.

2. Mean-field approximation

For simplicity, we limit the consideration to the isotropic Heisenberg model in an external field:

$$\mathcal{H} = -\frac{1}{2}\sum_{fg} J_{fg}\vec{S}_f\vec{S}_g - H\sum_f S_f^z,$$

where $\{f, g\}$ are the lattice indices. In the mean-field approximation, the energy and free energy are

$$W = -\frac{1}{2}\sum_{fg} J_{fg}\sigma_f\sigma_g\left(\cos(\theta_f)\cos(\theta_g) + \sin(\theta_f)\sin(\theta_g)\cos(\varphi_f-\varphi_g)\right) - H\sum_f \sigma_f\cos(\theta_f)$$

$$F = W + \sum_f\left[H_f\sigma_f - T\ln\left(2\cosh(H_f/2T)\right)\right],$$

where σ_f is the spin magnetization in the f position, $H_f = -\partial W/\partial\sigma_f$ is the effective field on this spin, θ_f and φ_f are the pointing angles of the spin with respect to the external magnetic field H, all the spins are equal to 1/2, and the Bohr magneton and Boltzmann and Planck constants are taken as units.

The above expression for W is simple enough to use in searching for a system state in the representation of two planar waves with wavevectors directed along the z-axis:

$$\sigma_{nf} = \sigma_n, \qquad \theta_{nf} = \theta_n, \qquad \varphi_{nf} = q_n z_{nf}, \qquad n = \{a, b\},$$

where z_f is the f component along the z-axis, n is the subsystem index. In the wave representation, the expression for the system

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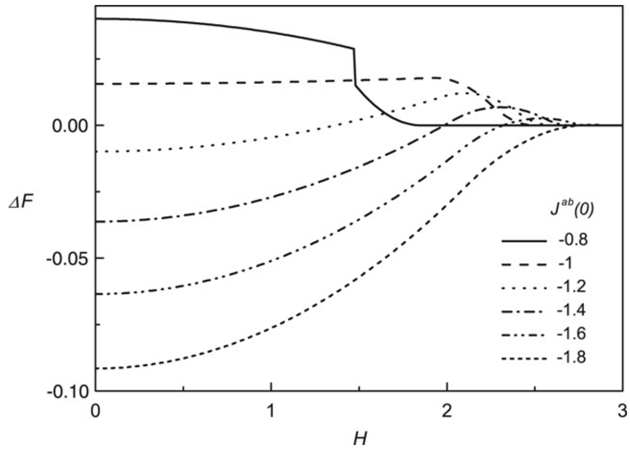

Fig. 1. Field dependence of the difference ΔF between the free energies of the incommensurable ($q_a = q_b$) and "semi-incommensurable" ($q_a \neq q_b$) states for several values of the integral $J^{ab}(0)$ at $T = 0$.

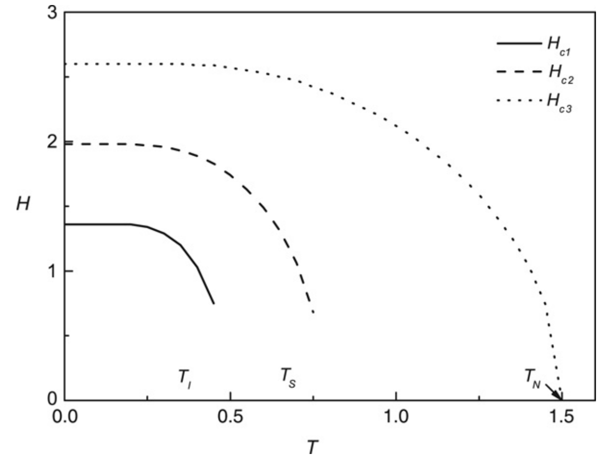

Fig. 2. Magnetic phase diagram of the model under consideration at $J^{ab}(0) = -1.2$.

energy is

$$\begin{aligned} W = N \Big\{ & -\frac{1}{2}\left(J^a(0)\cos^2(\theta_a) + J^a(q_a)\sin^2(\theta_a)\right)\sigma_a^2 \\ & -\frac{1}{2}\left(J^b(0)\cos^2(\theta_b) + J^b(q_b)\sin^2(\theta_b)\right)\sigma_b^2 \\ & - \big(J^{ab}(0)\cos(\theta_a)\cos(\theta_b) \\ & + J^{ab}(q_a)\sin(\theta_b)\sin(\theta_b)\delta_{q_a q_b}\big)\sigma_a\sigma_b \\ & - H\left(\sigma_a\cos(\theta_a) + \sigma_b\cos(\theta_b)\right)\Big\}, \end{aligned}$$

where $N = \sum_f 1$, $\delta_{q_a q_b}$ is the Kronecker symbol.

3. Numerical analysis

In the absence of interaction between the subsystems, each of them is ordered with its own wavevector; if this interaction is sufficiently strong, the system is ordered with a common wavevector. Having minimized the free energy via the system parameters, we analyzed numerically the changes in the ordering character depending on the integral of exchange interaction between the subsystems and on the external field. For this purpose, the parameters were specified as follows:

$$J^a(q) = 4 - 2\cos(q), \qquad J^b(q) = 2 - \cos(q) - \cos(2q),$$
$$J^{ab}(q) = J^{ab}(0)\cos(q/2).$$

The dispersion form of the last interaction is related to (caused by) its frustration in the commensurable phase of the copper metaborate, $J^{ab}(\pi) = 0$.

One can see in Fig. 1 that the low-field part of the $\Delta F(H)$ dependence changes faster with $J^{ab}(0)$ as compared to the high-field part; this causes non-monotone field behavior of the difference of free energy of the system under analysis in a certain region of values of this exchange integral. As a result, in the field satisfying the equality $\Delta F(H) = 0$ a first-order phase transition from an incommensurable to a "semi-incommensurable" state should occur.

Fig. 2 presents a calculated magnetic diagram of the model under consideration at $J^{ab}(0) = -1.2$. With increasing of the external field H, the sequence of changing phases is as follows: (1) up to the first critical field H_{c1} the incommensurable state is stable; (2) at $H = H_{c1}$, as a result of the first-order phase transition, the spin system changes its state to a "semi-incommensurable" one; (3) at the second critical field H_{c2}, spins of the b-subsystem collapse ($\theta_a \neq 0, \theta_b = 0$); (4) at the third critical field H_{c3} spins of the a-subsystem collapse ($\theta_a = 0, \theta_b = 0$).

In the copper metaborate phase diagrams obtained using a few different experimental methods, the boundary between the incommensurable and "semi-incommensurable" phases in the temperature region (T_I, T_S) is absent [4]. Therefore, it would be useful to carry out measurements which would complete this diagram.

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