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MAGNETIC-FIELD-INDUCED LONG-RANGE ANTIFERROMAGNETIC ORDER IN TWO-DIMENSIONAL FRUSTRATED SPIN-1/2 SYSTEMS

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One generally believes that in frustrated 2D spin-1/2 antiferromagnets the long-range antiferromagnetic order may be absent due to the quantum spin fluctuations. A relatively weak magnetic field may induce the canted antiferromagnetic ordering instead of the usuall one sublattice magnetic ordering.

The problem of the long-range antiferromagnetic (AFM) order in two-dimensional spin-1/2 Heisenberg frustrated systems draws much attention because its relevance for high-T_c superconductors. Usually one takes into account the exchange integrals J_1 and J_2 between the first and second neighbours, chosen to be positive for the AFM exchange, and considers a square lattice of spins. If one treats the spins as classical vectors, then at $J_1 > 2J_2$ the staggered AFM structure with the wave vector $\mathbf{Q} = (\pi, \pi)$ should realize, and at $J_1 < 2J_2$ the stripe ordering with $\mathbf{Q} = (0, \pi)$.

But, as well known, the classical AFM ordering is not an exact eigenstate of the Heisenberg Hamiltonian, and the spins display the zero-point spin-oscillations. Even in absence of frustrations their amplitude in a 2D $S = 1/2$ antiferromagnet is so large that the question arises whether the AFM long-range order (LRO) exists in them. An analysis carried out in [1] evidences that, apparently, it does exist though the energy difference between the AFM ordered and disordered RVB states is negligible. In this case the standard spin-wave approximation yields unexpectedly accurate estimates for the mean spin M and the ground state energy, the former being very close to experimental values of mean spins in high-T_c superconductors.

If the case of $J_2 = 0$ is marginal, much more suspicious in this respect is the case of J_2 close to $2J_1$ when the role of spin fluctuations is still more enhanced. This is a consequence of the fact that exchanges between the first and second nearest neighbours tend to establish different types of magnetic ordering and for this reason interfere with each other. As was shown in [2] basing on the usual spin-wave approximation and Bogolyubov transformation of operators of spin deviations $b_{\mathbf{q}} = u_{\mathbf{q}}\beta_{\mathbf{q}} + v_{-\mathbf{q}}\beta^{+}_{-\mathbf{q}}$, the mean spin $M = 1/2 - 1/N\sum|v_{\mathbf{q}}|^2$ turns out to be negative in the vicinity of the phase boundary $J_1 = 2J_2$. The conclusion that the long-range order (LRO) should be absent there was made in [2] though, strictly speaking, this means only inapplicability of the spin-wave approximation.

Subsequent investigations were not convincing enough to support or to reject unambiguously the idea of disappearance of the LRO (see their review in [3]). Nevertheless, keeping in mind the marginal character of the AFM LRO at $J_2 = 0$, we believe that the opinion that it is absent at $J_1 \approx 2J_2$ is quite reasonable.

If the AFM LRO is really absent, the idea arises, that the AFM ordering can appear in an external magnetic field since the latter causes the spin canting and, hence, diminishes the amplitude of the zero-point spin fluctuations (in the spin-flopped state they are absent at all). Then the magnetic field, in addition to the standard magnetization, can produce an unstandard effect: it can induce the AFM ordering. Judging from the fact that the magnetic anisotropy by itself can suppress the LRO window, returning the system to the classical AFM ordering specific for the Ising model, one may conclude that its presence can drastically reduce the field strength at which the LRO appears.

One considers a square lattice of spin-1/2 magnetic atoms in the (xy) plane, the x axis being the easy axis. The magnetic field is perpendicular to the (xy) plane. The Hamiltonian of the system under consideration is

$$\hat{H} = \frac{1}{2}\sum_{\xi,\mathbf{g},\Delta} J_1^{\xi} S_{\mathbf{g}}^{\xi} S_{\mathbf{g}+\Delta}^{\xi} + \frac{1}{2}\sum_{\xi,\mathbf{g},\delta} J_2^{\xi} S_{\mathbf{g}}^{\xi} S_{\mathbf{g}+\delta}^{\xi} - H\sum_{\mathbf{g}} S_{\mathbf{g}}^{z}, \qquad (1)$$

where $S_{\mathbf{g}}^{\xi}$ is the spin projection of atom $\mathbf{g} = (g_x, g_y)$ onto the ξ-axis ($\xi = x, y$ or z). Vectors Δ and δ connect the first and second nearest neighbours, respectively. The magnetic anisotropy corresponds to the anisotropy of the exchange integrals $J_i^y = J_i^z = J_i$, $J_i^x = \mu J_i$ with anisotropy parameter μ exceeding 1 ($i = 1, 2$).

As the aim of the present investigation is to obtain only semiquantitative results, we use the most simplest version of the theory leading to the LRO window at $H = 0$ – the standard spin-wave approximation of [1]. The more, we are unable to decide which numerical results concerning the width of the window are the most reliable since the accuracy of all the approximations described in [3] is uncontrollable in the absence of a small parameter.

The procedure of using the spin-wave approximation in an AFM system canted by an external magnetic field is described in [4] in detail. One introduces local reference frames $(x_{\mathbf{g}}, y_{\mathbf{g}}, z_{\mathbf{g}})$ for each atom $\mathbf{g}$ in such a way that the $z_{\mathbf{g}}$ axis coincides with the direction of the sublattice moment for atom $\mathbf{g}$ and the $y_{\mathbf{g}}$ axis coincides with the y axis in the laboratory frame of reference. Then one uses the Holstein – Primakoff transformation from the spin component to the magnon operators $b_{\mathbf{g}}^{+}$, $b_{\mathbf{g}}$ in the local frame:

$$S^{x\mathbf{g}}_{\mathbf{g}} = \frac{1}{2}(b^+_{\mathbf{g}} + b_{\mathbf{g}}) = S^x_{\mathbf{g}} \cos\Theta - S^z_{\mathbf{g}} \sin\Theta e^{i\mathbf{Q}\mathbf{g}},$$

$$S^{y\mathbf{g}}_{\mathbf{g}} = \frac{i}{2}(b^+_{\mathbf{g}} - b_{\mathbf{g}}) = S^y_{\mathbf{g}}, \tag{2}$$

$$S^{z\mathbf{g}}_{\mathbf{g}} = \frac{1}{2} - b^+_{\mathbf{g}} b_{\mathbf{g}} = S^x_{\mathbf{g}} \sin\Theta e^{i\mathbf{Q}\mathbf{g}} + S^z_{\mathbf{g}} \cos\Theta,$$

where Q is the antiferromagnetic vector of the ordered state. The angle $\pm\Theta$ between the z axis and $z_{\mathbf{g}}$ axis is determined from the condition of the minimum classical E_0 energy obtained after substituting (2) in (1) (this condition coincides with the disappearance condition for terms linear in magnon operators):

$$\cos\Theta = h = \frac{H}{H_c}, \tag{3}$$

where H_c is the spin-flop field. The expressions for H_c and E_0 in the staggered Néel phase are as follows:

$$H^N_c = 2J_1(1 + \mu - \alpha(\mu - 1)), \tag{4}$$

$$E^N_0 = -\frac{N}{2}(\mu(J_1 - J_2) + J_1(1 + \mu - \alpha(\mu - 1))h^2) \tag{5}$$

and for the stripe Landau phase:

$$H^L_c = 2J_1(1 + \alpha(\mu + 1)), \tag{6}$$

$$E^L_0 = -\frac{N}{2}(\mu J_2 + J_1(1 + \alpha(\mu + 1))h^2) \tag{7}$$

with N being the number of atoms and $\alpha = J_2/J_1$. Equating E^N_0 (5) and E^L_0 (7), one obtains the classical boundary α_b between phases as a function of μ and h.

The magnon spectrum is found through the Bogolyubov transformation of the boson operators in (1)–(3):

$$\omega(\mathbf{q}) = 4J_1\sqrt{A^2_{\mathbf{q}} - B^2_{\mathbf{q}}}, \tag{8}$$

where for the Néel phase:

$$A^N_{\mathbf{q}} = \mu(1 - \alpha) + \alpha\left(1 + \frac{\mu - 1}{2}h^2\right)\gamma_{\mathbf{q}d} + \frac{1 + \mu}{2}h^2\gamma_{\mathbf{q}g},$$

$$B^N_{\mathbf{q}} = \left(\frac{1 + \mu}{2}h^2 - 1\right)\gamma_{\mathbf{q}g} + \alpha\frac{\mu - 1}{2}h^2\gamma_{\mathbf{q}d} \tag{9}$$

and for Landau phase:

$$A^L_{\mathbf{q}} = \left(\frac{1}{2} + \frac{\mu - 1}{4}h^2\right)\gamma_{\mathbf{q}y} + \frac{\mu + 1}{4}h^2\gamma_{\mathbf{q}x} + \alpha\left(\mu + \frac{\mu + 1}{2}h^2\gamma_{\mathbf{q}d}\right),$$

$$B^L_{\mathbf{q}} = \frac{\mu - 1}{4}h^2\gamma_{\mathbf{q}y} + \left(\frac{\mu + 1}{4}h^2 - \frac{1}{2}\right)\gamma_{\mathbf{q}x} + \alpha\left(\frac{\mu + 1}{2}h^2 - 1\right)\gamma_{\mathbf{q}d}, \tag{10}$$

$$\gamma_{\mathbf{q}x} = \cos(q_x), \quad \gamma_{\mathbf{q}y} = \cos(q_y), \quad \gamma_{\mathbf{q}g} = \frac{1}{2}(\gamma_{\mathbf{q}x} + \gamma_{\mathbf{q}y}), \quad \gamma_{\mathbf{q}d} = \gamma_{\mathbf{q}x}\gamma_{\mathbf{q}y}.$$

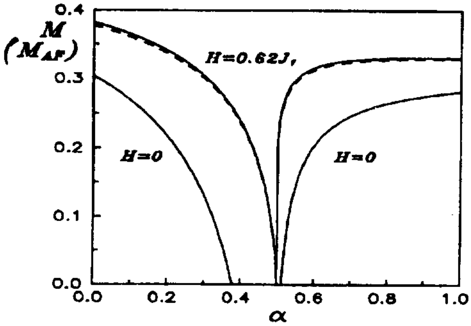

Fig.1. Dependence of magnetic moment M (solid lines) and its AFM component M_{AF} (dotted lines) on the frustration parameter α at $H = 0$ and $H = 0.62J_1$ and zero anisotropy

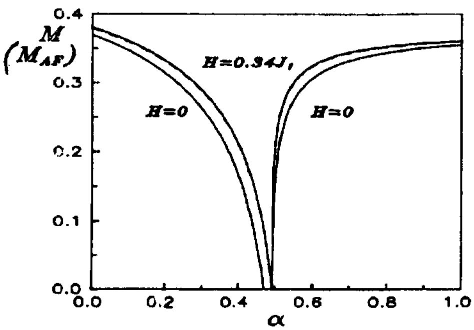

Fig.2

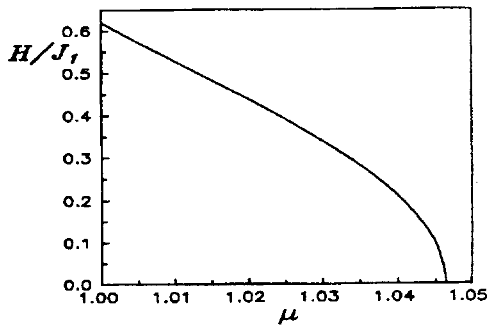

Fig.3.

Fig.2. Dependence of magnetic moment M (solid lines) and its AFM component M_{AF} (dotted lines) on the frustration parameter α at $H = 0$ and $H = 0.34J_1$ and anisotropy of 3%

Fig.3. Dependence of the window closing field on the anisotropy μ

The average moment M at $T = 0$ is given by the expression

$$M = \langle S^{z\mathrm{g}}_{\mathrm{g}} \rangle = \frac{1}{2} - \langle b^{+}_{\mathrm{g}} b_{\mathrm{g}} \rangle = 1 - \frac{2J_1}{N} \sum_{\mathrm{q}} \frac{A_{\mathrm{q}}}{\omega(\mathrm{q})}. \tag{11}$$

The summation over q runs over the Brillouin zone.

First, the role of magnetic anisotropy at $H = 0$ will be discussed. As follows from (11), the LRO window disappears at $\mu = 1.045$. Thus, the effect considered by us should realize at the anisotropy less than 5%. In Fig.1 the magnetization per atom M and its AFM component $M_{AF} = M \sin\Theta$ are represented for an isotropic system ($\mu = 1$) as a function of the frustration parameter. As seen from it, the quantum fluctuations influence the staggered LRO much stronger than the stripe LRO: the window at $H = 0$ is located between α values of 0.38 and 0.51. But in the field of $0.62J_1$ (which corresponds to $0.155H_c$) the window becomes closed. According to Fig.2 at nonzero anisotropy (3%) the window for $H = 0$ is much more narrow, and it is closed already at a field of $0.34J_1$ (i.e. of $0.084H_c$). Dependence of the window-closing magnetic field on the magnetic anisotropy is presented in Fig.3.

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