Magnetic-field induced long-range antiferromagnetic order in two-dimensional frustrated spin-1/2 systems

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It is generally believed that in frustrated two-dimensional spin-1/2 antiferromagnets the long-range antiferromagnetic order may be absent because of quantum spin fluctuations. A relatively weak magnetic field may induce the canted antiferromagnetic ordering instead of the usual one-sublattice magnetic ordering. © *1995 American Institute of Physics.*

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

But, as is well known, the classical AFM ordering is not an exact eigenstate of the Heisenberg Hamiltonian, and the spins exhibit zero-point spin oscillations. Even in absence of frustration their amplitude in a 2D $S=1/2$ antiferromagnet is so large that the question arises of whether AFM long-range order (LRO) exists in them. An analysis carried out in Ref. 1 suggests that it apparently does exist, even though the energy difference between the antiferromagnetically 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 the experimental values of the mean spins in high-T_c superconductors.

While the case $J_2=0$ is marginal, much more suspicious in this respect is the case of J_2 close to $2J_1$, where the role of spin fluctuations is still more enhanced. This is a consequence of the fact that the exchanges between the first and second nearest neighbors tend to establish different types of magnetic ordering and for this reason interfere with each other. As was shown in Ref. 2 on the basis of the usual spin-wave approximation and Bogolyubov transformation of the spin-deviation operators $b_{\mathbf{q}} = u_{\mathbf{q}}\beta_{\mathbf{q}} + v_{-\mathbf{q}}\beta^{+}_{-\mathbf{q}}$, the mean spin $M = 1/2 - 1/N\Sigma|v_{\mathbf{q}}|^2$ 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 Ref. 2, although strictly speaking, this only means that the spin-wave approximation is inapplicable there.

Subsequent investigations were not convincing enough to support or to reject unambiguously the idea of vanishing of the LRO (see the review in Ref. 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 AFM ordering may appear in an external magnetic field, since the latter causes spin canting and, hence, diminishes the amplitude of the zero-point spin fluctuations (in the spin-flopped state they are completely absent). Then a magnetic field, in addition to the standard magnetization, can produce a nonstandard effect: it can induce 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 to 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

$$\tilde{H}=\frac{1}{2}\sum_{\xi,\mathbf{g},\Delta} J_1^{\xi} S_{\mathbf{g}}^{\xi} S_{\mathbf{g}+\Delta}^{\xi}+\frac{1}{2}\sum_{\xi,\mathbf{g},\delta} J_2^{\xi} S_{\mathbf{g}}^{\xi} S_{\mathbf{g}+\delta}^{\xi}-H\sum_{\mathbf{g}} S_{\mathbf{g}}^{z}, \tag{1}$$

where $S_{\mathbf{g}}^{\xi}$ is the spin projection of the atom $\mathbf{g} = (g_x, g_y)$ onto the ξ axis ($\xi=x,y$ or z) Vectors $\boldsymbol{\Delta}$ and $\boldsymbol{\delta}$ connect the first and second nearest neighbors, 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 the anisotropy parameter μ exceeding 1 ($i=1,2$).

As the aim of the present investigation is to obtain only semiquantitative results, we use the simplest version of the theory which leads to the LRO window at $H=0$—the standard spin-wave approximation of Ref. 1. Moreover, 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 Ref. 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 detail in Ref. 4 One introduces local reference frames $(x_{\mathbf{g}}, y_{\mathbf{g}}, z_{\mathbf{g}})$ for each atom **g** in such a way that the $z_{\mathbf{g}}$ axis coincides with the direction of the sublattice moment for atom **g** and the $y_{\mathbf{g}}$ axis coincides with the **y** axis in the laboratory reference frame. 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:

$$S_{\mathbf{g}}^{x_{\mathbf{g}}}=\tfrac{1}{2}(b_{\mathbf{g}}^{+}+b_{\mathbf{g}})=S_{\mathbf{g}}^{x}\cos\Theta-S_{\mathbf{g}}^{x}\sin\Theta e^{i\mathbf{Qg}},\quad S_{\mathbf{g}}^{y_{\mathbf{g}}}=\frac{i}{2}(b_{\mathbf{g}}^{+}-b_{\mathbf{g}})=S_{\mathbf{g}}^{y}, \tag{2}$$

$$S_{\mathbf{g}}^{z_{\mathbf{g}}}=\tfrac{1}{2}-b_{\mathbf{g}}^{+}b_{\mathbf{g}}=S_{\mathbf{g}}^{x}\sin\Theta e^{i\mathbf{Qg}}+S_{\mathbf{g}}^{z}\cos\Theta,$$

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 minimum classical energy E_0 obtained after substituting (2) in (1) (this condition coincides with the condition that terms linear in the magnon operators vanish):

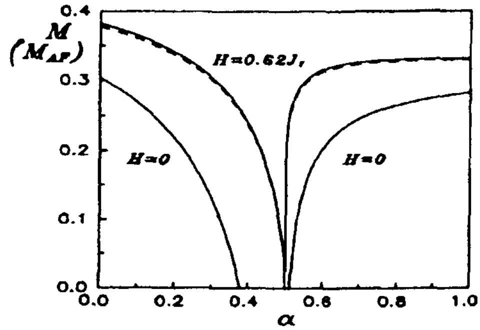

FIG. 1. Dependence of the magnetic moment M (solid curves) and its AFM component M_{AF} (dashed curves) on the frustration parameter α at $H=0$ and $H=0.62J_1$ for zero anisotropy.

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

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

$$H_c^N = 2J_1[1+\mu-\alpha(\mu-1)], \tag{4}$$

$$E_0^N = -\frac{N}{2}(\mu(J_1-J_2)+J_1[1+\mu-\alpha(\mu-1)]h^2) \tag{5}$$

and for the stripe Landau phase

$$H_c^L = 2J_1[1+\alpha(\mu+1)], \tag{6}$$

$$E_0^L = -\frac{N}{2}[\mu J_2 + J_1[1+\alpha(\mu+1)]h^2] \tag{7}$$

with N being the number of atoms and $\alpha = J_2/J_1$. Equating E_0^N (5) and E_0^L (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):

$$\omega(\mathbf{q}) = 4J_1\sqrt{A_{\mathbf{q}}^2 - B_{\mathbf{q}}^2}, \tag{8}$$

where for the Néel phase:

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

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

and for Landau phase:

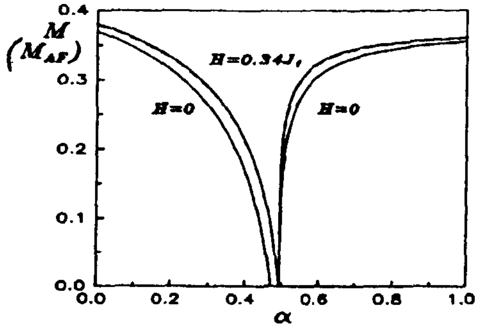

FIG. 2. Dependence of the magnetic moment M (solid curves) and its AFM component M_{AF} (dashed curves) on the frustration parameter α at $H=0$ and $H=0.34\ J_1$ for an anisotropy of 3%.

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

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

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

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

$$M=(S_{\mathbf{g}}^{z_{\mathbf{g}}})=\frac{1}{2}-\langle b_{\mathbf{g}}^{+}b_{\mathbf{g}}\rangle=1-\frac{2J_1}{N}\sum_{\mathbf{q}}\frac{A_{\mathbf{q}}}{\omega(\mathbf{q})}. \tag{11}$$

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 be realized for an anisotropy less than 5%. In Fig. 1 the magnetization per atom M and

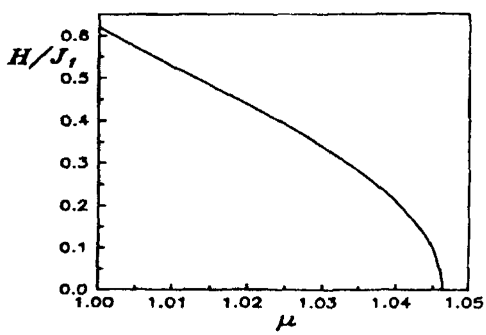

FIG. 3. Dependence of the window-closing field on the anisotropy μ.

its AFM component $M_{AF} = M\sin\Theta$ are represented for an isotropic system ($\mu=1$) as a function of the frustration parameter. It is seen that the quantum fluctuations influence the staggered LRO much more strongly than the stripe LRO: the window at $H=0$ is located between α values of 0.38 and 0.51. But in a field of 0.62 J_1 (which corresponds to $0.155H_c$) the window becomes closed. According to Fig. 2, at nonzero anisotropy (3%) the window at $H=0$ is much more narrow, and it is closed completely at a field of only $0.34J_1$ (i.e., $0.084H_c$). The dependence of the window-closing magnetic field on the magnetic anisotropy is presented in Fig. 3.

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