Orientational transitions in Heisenberg antiferromagnets on triangular lattice

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In 2D-isotropic hexagonal Heisenberg antiferromagnets, the spin flip in a magnetic field occurs through an intermediate phase with an unbroken, continuous symmetry and with a constant magnetization equal to 1/3 of the nominal value. In strong fields the noncollinear phase is characterized by a parallel arrangement of the spins of the two sublattices and by a nonvanishing transverse magnetization.

1. The research interest in the properties of 2D antiferromagnets on a triangular lattice can be credited to a large extent to the discussion by Anderson and Fazekas[1,2] of the possibility of realizing a nonmagnetic ground state for an antiferromagnet on a triangular lattice with $S = 1/2$ as a result of *numerically* large zero-point vibrations. Our purpose in the present letter is to show that the 2D nature of the problem also leads to several fundamental effects which are unrelated to the small value of S: Regardless of the size of the spin, a spin flip in an external magnetic field at $T = 0$ occurs through a collinear intermediate phase with a fixed magnetization equal to 1/3 of the nominal value. The possibility of a nontrivial behavior stems from the existence of an additional "random" degeneracy at the classical level of the analysis in the 2D case[3]: A state of a triad of classical spins is described by three angle equations in either a zero or nonzero magnetic field. As a result, the excitation spectrum constructed above the "natural" ground state (all the spins make the same angle with the field direction, and their projections onto the plane perpendicular to the field form a 120° star) contains, in addition to the ordinary branch which is linear in $|k|$ and a branch with $\omega(k=0) \equiv vH$, an additional gapless branch of excitations with $\omega \sim k^2$. As a result, some different and fairly exotic states have the same energy as the natural state in the classical treatment, and the choice of ground state is dictated by quantum fluctuations.[1)]

2. Among the states with the minimum classical energy we select a configuration in which the spins remain in a common plane in the course of the spin flip. This plane passes through the axis singled out by the field, and the reorientation process plays out as shown in Fig. 1. According to the classical treatment, a phase transition occurs (two sublattices collapse) in a configuration of this sort in a field $H_c = H_{sat}/3$ ($H_{sat} = 18J'S$, where J' is the exchange integral for nearest neighbors). Associated with this phase transition is an additional softening of the spectrum: The two gapless excitation modes above the collinear state in Fig. 1 ($H = H_c$) turn out to be quadratic in the wave vector. The existence of this additional softness in the spectrum constructed above the classical ground state suggests that this spin-flip process corresponds to the minimum energy of a real quantum system. A direct calculation of the energy of the zero-point vibrations through a $1/S$ expansion confirms this suggestion: A spin flip in the isotropic case does indeed occur as shown in Fig. 1.

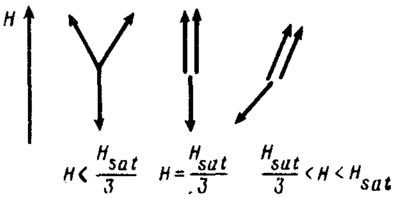

FIG. 1. That reorientation process in a magnetic field which corresponds to the ground state of the quantum system. Zero-point vibrations stabilize the collinear phase in the finite field interval $H_1 < H < H_2$ near $H_{sat}/3$.

Furthermore, a calculation shows that in a quantum system a collinear phase exists in a *finite* field interval $H_1 < H < H_2$. In first order in the reciprocal of the spin we have

$$\Delta H = H_2 - H_1 = \left(\frac{H_{sat}}{3}\right) \frac{2}{S} \sum_{\mathbf{k}} \frac{(1+\epsilon_3)(\epsilon_3 - \epsilon_1\epsilon_2)}{(\epsilon_1+\epsilon_3)(\epsilon_2+\epsilon_3)}, \tag{1}$$

where ε_i are the real, positive classical frequencies of the three branches of one-particle excitations, and ε_1, ε_2, and $-\varepsilon_3$ are the roots of the equation.

$$\begin{gathered} \epsilon^3 - \epsilon^2 - \epsilon\,(1 - |\nu_{\mathbf{k}}|^2) + 1 + \nu_{\mathbf{k}}^3 + \nu_{-\mathbf{k}}^3 - 3|\nu_{\mathbf{k}}|^2 = 0; \\ \nu_{\mathbf{k}} = \frac{1}{3}\left(e^{ik_x} + e^{ik_y} + e^{-i(k_x+k_y)}\right). \end{gathered} \tag{2}$$

It is easy to verify [even without solving (2) explicitly] that ΔH is definitely positive. The expressions for the critical fields H_1 and H_2 themselves are rather lengthy, and we will not reproduce them here. The absence of a spontaneous breaking of the continuous symmetry in the collinear phase (the space of the order parameter $V = Z_3$) has the consequence that all the resonant frequencies have a finite gap. According to a calculation, in the interval $H_1 < H < H_2$ we have

$$\omega_1 \equiv \gamma H, \quad \omega_3 \approx \gamma(H_2 - H), \quad \omega_2 \approx \gamma(H - H_1). \tag{3}$$

Note that we have $\omega_{2,3} \sim 1/S$. The ground state is nondegenerate, so the magnetization is constant in the interval ΔH. The zero-point vibrations *do not* change the classical value $M = M_{sat}/3$ (at least in first order in $1/S$).

The region of the collinear phase has a finite width because of the difference in the types of transitions at $H = H_1$ and $H = H_2$: In addition to the breaking of the continuous symmetry which is common to the two cases, the transition at $H = H_2$ is characterized by the nucleation of a *transverse* magnetization $M_\perp$, with

$$M_\perp \sim \frac{1}{S}(H - H_2)^{1/2}, \quad H \gtrsim H_2 \tag{4}$$

Figure 2 shows the behavior of $\mathbf{M}(H)$.

3. A specific feature of the 2D case from the macroscopic standpoint results from

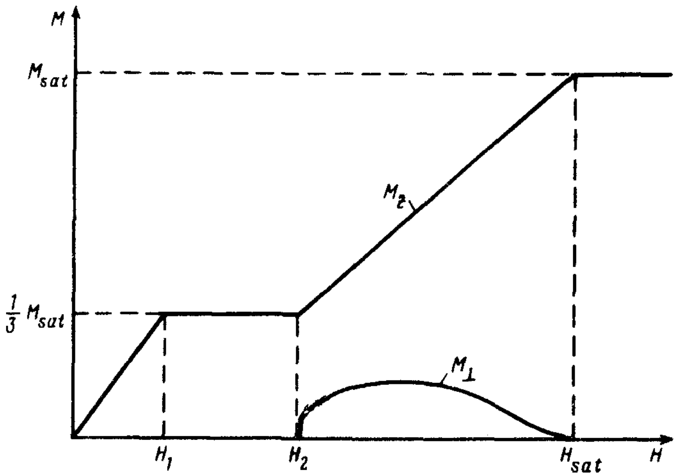

FIG. 2.

the vanishing of the quantity $\eta = \chi_{\parallel} - \chi_{\perp}/\chi_{\perp}$, which, according to Ref. 7, determines one of the resonant frequencies in the 3D systems: $\omega_3 = \eta H$. Correspondingly, the quantum gap, which singles out the planar configuration in Fig. 1 in the 2D case, is proportional to the cube of the magnetic field in weak fields. As a consequence, in a quasi-2D antiferromagnetic system on a triangular lattice (a stack of hexagonal planes) the spin flip begins in the usual way,[8] and the phase transition to the planar configuration occurs at $H \sim H_{sat}(S_\eta)^{1/2}$.

4. A corresponding effect occurs in a classical system ($S = \infty$), when there is an easy-axis anisotropy, since the field of the spin-flip transition formally becomes infinite in the 2D case.[9]

The spin flip occurs as in Fig. 1. The collinear phase is again realized in a finite field interval

$$H_1 < H < H_2, \quad H_1 \equiv 6J'S\left(1 - \frac{\tilde{D}}{3J'}\right), \; H_2 \approx 6J'S\left(1 + \frac{\tilde{D}}{J'}\right), \qquad H_{sat} = 18J'S\left(1 - \frac{\tilde{D}}{9J'}\right) \tag{5}$$

(the notation here is the same as that of Ref. 9). Furthermore, we have

$$M_\perp = \mu S\left(\frac{\tilde{D}}{24J'}\right) \begin{cases} \frac{32}{3}\left(\frac{H}{H_2} - 1\right)^{1/2}, & H \gtrsim H_2 \\ \frac{8}{9\sqrt{3}}\left(1 - \frac{H}{H_{sat}}\right)^{3/2}, & H \lesssim H_{sat}. \end{cases} \tag{5'}$$

The only distinction from the isotropic case is that with an anisotropy two of the three resonant frequencies are nonzero even at $H = 0$.

5. A random degeneracy at the classical level also prevails in easy-plane systems, but in a field which is directed in the easy plane. The simplest example here is the XY model.[10-12] It was shown in Refs. 11 and 12 that incorporating thermal fluctuations in the limit $T \Rightarrow +0$ introduces the condition on the angles which we need, and the spin flip again occurs as in Fig. 1 (the XY plane is the plane of the figure). We have carried out calculations at $T=0$ for a quantum system, and we have found that the zero-point vibrations also fix the state shown in Fig. 1 as the ground state. Again, the collinear phase exists in a *finite* field interval

$$\Delta H = H_2 - H_1 = \left(\frac{H_{sat}}{3}\right) \frac{1}{S} \sum_{\mathbf{k}} \frac{(\omega_{\mathbf{k}} - 1)^2(\omega_{\mathbf{k}} + 1)}{\omega_{\mathbf{k}}} > 0, \tag{6}$$

where $\omega_k = 1 + \nu_k + \nu_{-k}$. Inside this interval, the ground state is nondegenerate, and all the excitations have a finite gap ($\omega_1 \approx \gamma H_{sat}/\sqrt{3}, \omega_2 \approx \gamma (H_{sat}/3(H-H_1))^{1/2}, \omega_3 = \gamma (H_{sat}/9(H_2 - H))^{1/2}$. It is true that, in contrast with the isotropic case, the magnetization is not constant in the collinear phase. The reason is that when the field is in the plane, the Hamiltonian of the XY model does not commute with the Z component of the total spin.

6. A finite region of a collinear phase in a classical isotropic system and in a classical XY system at $T \neq 0$ has been seen in numerical simulations.[3,10,13] We wish to assert that in the corresponding quantum systems this region will also be finite at $T=0$. Furthermore, the corresponding field interval ΔH will not be at all small in the general case of an arbitrary spin. Experimentally, a plateau on the $M(H)$ curve at the level of $(1/3)M_{sat}$ has been observed as $T \Rightarrow 0$ in C_6Eu samples during the application of a field in the easy plane (a system with XY symmetry). The field interval ΔH was fairly wide ($H_1 \approx 22$kOe, $H_2 \approx 82$ kOe with $H_{sat} \approx 205$ kOe).[14]

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[1)] Here we are seeing a realization of the principle of "order through disorder,"[4] since the presence of a mode which is quadratic in k leads at the formal level to a blurring of the long-range order in the 2D case. A situation of this sort is typical of several 2D systems with competing interactions.[5,6]

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