Triangular planar antiferromagnet in an external magnetic field

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The triangular planar antiferromagnet (TPA) in an external magnetic field H is widely studied both analytically and numerically. Low-temperature expansion of the free energy shows that the infinite degeneracy of the minimum-energy configurations is lifted by thermal fluctuations and Monte Carlo simulation provides a rich phase diagram in the H-T plane where three different configurations are encircled by the paramagnetic saturated phase. Here, we give explicitly the elementary excitation dispersion curves. The field dependence of the uniform modes is closely related to the minimum-energy configuration selected by thermal fluctuations. Some real compounds are indicated as possible candidates to test experimentally the phenomenology of the TPA model. We have also explained the stability over a finite region in the H-T plane of the phase characterized by two spins parallel and one spin antiparallel to the field in the magnetic cell. The stabilizing mechanism of this phase arises from crucial nonlinear effects. For this phase the presence of long-range order is proven analytically.

I. INTRODUCTION

The misfit between antiferromagnetism and triangular structure is a well-known source of interesting frustration phenomena. A classical example where this frustration is found is the Ising triangular antiferromagnet, which was solved exactly by Wannier.[1] This model shows a behavior quite different from the square Ising antiferromagnet where a second-order phase transition is found.[2] Indeed, the triangular Ising antiferromagnet is disordered not only at any finite temperature but even at zero temperature with a finite entropy $S(0) = 0.3231R$.[1] As concerns the continuous symmetry models such as planar, XY, and Heisenberg models, long-range order (LRO) is prevented at any finite temperature for any 1D and 2D lattice structure on the basis of the well-known Mermin and Wagner theorem.[3] The triangular planar antiferromagnet (TPA) has been extensively studied by both Monte Carlo (MC) simulations[4,5] and analytic low-temperature expansions[6,7] in zero and finite external magnetic field.

An interesting phase diagram is suggested by MC simulations.[4,5] Some remarkable features of the phase diagram are (i) the lifting at finite temperature of the infinite degeneracy, which is present at zero temperature at any magnetic field, and (ii) a sequence of three ordered phases at fixed temperature as the magnetic field is increased until the saturated paramagnetic phase is reached.

The analytic approach to the TPA (Refs. 6 and 7) consists of a low-temperature expansion of the free energy, the leading term of which is given by the harmonic approximation. The so-obtained harmonic free energy selects a configuration with the spins of the three sublattices forming an angle of nearly 120° at low field, with one spin opposite to the field.[6,7] In contrast, in Fig. 2 of Ref. 4 the suggested configuration is a nearly 120° configuration with one spin pointing along the field. The same assumption about the ground-state configuration was recently performed[8] to explain the magnetic-resonance experimental data concerning $CsCuCl_3$ in an external magnetic field. This magnetic insulator consists of weakly interacting spin chains crossing the c plane according to a triangular lattice. An easy plane anisotropy is present so that the Hamiltonian model shows an XY symmetry. We notice that the behavior of the uniform modes in an external magnetic field perpendicular to the chains is strongly dependent on the actual ground-state configuration. In particular, crossings between the resonance frequencies are expected for the ground-state configuration assumed in Ref. 8, at variance with the experiment. In contrast, no crossing occurs if the ground state pointed out in Refs. 6 and 7 is assumed. We stress that magnetic-resonance experiment in this and related compounds of the hexagonal ABX_3-type should be interesting tests of the rich phenomenology related to the frustration of the TPA model.

In Sec. II we give explicitly the dispersion curves of the elementary excitations of the TPA model for selected values of the magnetic field. Moreover, we prove that nonlinear contributions to the free energy explain the stability over a finite region in the H-T plane of the configuration we call "up-up-down" phase where two spins of the magnetic cell are parallel and the third spin is opposite to the field.

In Sec. III we give analytic support to the existence of genuine LRO in agreement with the indications obtained by MC simulation.[4] We have also performed MC calculations for temperatures lower than those explored in literature in order to test the agreement between the low-temperature analytic results with the intermediate-temperature numerical calculations.

II. ELEMENTARY EXCITATIONS AND CRUCIAL NONLINEAR EFFECTS

The Hamiltonian of the model is

$$\mathcal{H} = 2J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j - \mu \mathbf{H} \cdot \sum_i \mathbf{S}_i, \qquad (1)$$

where i labels the sites of a triangular lattice, $< ij >$ means distinct nearest-neighbor (NN) pairs of two-dimensional spins, $2J$ is the exchange coupling, μ is the magnetic moment of a spin, $\mathbf{H}$ is the external magnetic field. Strictly following Refs. 6 and 7 we divide the triangular lattice in three sublattices on which the spins are supposed to form angles $\phi_1 + \psi_i^{(1)}$, $\phi_2 + \psi_i^{(2)}$, $\phi_3 + \psi_i^{(3)}$ with the external magnetic field. ϕ_1, ϕ_2, ϕ_3 are the angles that the spins of each sublattice form with the external magnetic field in the minimum free-energy configuration. $\psi_i^{(s)}(s = 1, 2, 3)$ are small deviations around the equilibrium configuration. If we expand Hamiltonian (1) in powers of $\psi_i^{(s)}$ we obtain

$$\mathcal{H} = E_0 + \sum_{n=2}^{\infty} \mathcal{H}_n, \tag{2}$$

where n labels the number of $\psi_i^{(s)}$ present in the Hamiltonian contribution $\mathcal{H}_n$. Minimization of E_0 with respect to ϕ_i , $i = 1, 2, 3$, gives the ground-state configuration[6,7]

$$\phi_1 = \phi \quad , \quad \phi_2 = \phi_\mp \quad , \quad \phi_3 = \phi_\pm, \tag{3}$$

where

$$\cos \phi_\mp = \frac{1}{2} \left[h - \cos \phi \mp \sin \phi \sqrt{(3 - h^2 + 2h \cos \phi)/(1 + h^2 - 2h \cos \phi)} \right],$$

$$\sin \phi_\mp = \frac{1}{2} \left[- \sin \phi \mp (h - \cos \phi) \sqrt{(3 - h^2 + 2h \cos \phi)/(1 + h^2 - 2h \cos \phi)} \right], \tag{4}$$

with $-\phi_M < \phi < \phi_M$, where $\phi_M = \pi$ for $0 < h < 1$, $\phi_M = \cos^{-1}[(h^2 - 3)/2h]$ for $1 < h < 3$ and $h = \mu H/6J$. As one can see from Eqs. (3) and (4) the ground state shows infinite degeneracy also in the presence of an external field.[4] Such configurations are explicitly given by Eqs. (3) and (4) for the first time. For $h \geq 3$ the minimum-energy configuration is unique and corresponds to the saturated phase $\phi_1 = \phi_2 = \phi_3 = 0$. The ground-state energy is independent of ϕ and reads

$$E_0 = -JN(3 + h^2) \tag{5}$$

for $0 \leq h \leq 3$ and

$$E_0 = 6JN(1 - h) \tag{6}$$

for $h > 3$. The first term of the sum appearing in Eq. (2) reads

$$\mathcal{H}_2 = 3J \sum_{s,s'=1}^{3} \sum_{\mathbf{q}} \psi_{-\mathbf{q}}^{(s)} A_{\mathbf{q}}^{ss'} \psi_{\mathbf{q}}^{(s')}, \tag{7}$$

where

$$\psi_{\mathbf{q}}^{(s)} = \frac{1}{\sqrt{N/3}} \sum_i \psi_i^{(s)} e^{-i\mathbf{q}\cdot\mathbf{r}_i}, \quad s = 1, 2, 3 \tag{8}$$

and

$$\mathbf{A_q} = \begin{pmatrix} 1 & \gamma_{\mathbf{q}} \cos(\phi_1 - \phi_2) & \gamma_{\mathbf{q}}^* \cos(\phi_1 - \phi_3) \\ \gamma_{\mathbf{q}}^* \cos(\phi_1 - \phi_2) & 1 & \gamma_{\mathbf{q}} \cos(\phi_2 - \phi_3) \\ \gamma_{\mathbf{q}} \cos(\phi_1 - \phi_3) & \gamma_{\mathbf{q}}^* \cos(\phi_2 - \phi_3) & 1 \end{pmatrix} \tag{9}$$

for $0 \leq h \leq 3$, and

$$\mathbf{A_q} = \begin{pmatrix} h-2 & \gamma_{\mathbf{q}} & \gamma_{\mathbf{q}}^* \\ \gamma_{\mathbf{q}}^* & h-2 & \gamma_{\mathbf{q}} \\ \gamma_{\mathbf{q}} & \gamma_{\mathbf{q}}^* & h-2 \end{pmatrix} \tag{10}$$

for $h > 3$. The structure factor reads

$$\gamma_{\mathbf{q}} = \frac{1}{3} \sum_{\delta} e^{i\mathbf{q}\cdot\delta} = \frac{1}{3} \left(e^{iq_x} + 2e^{-iq_x/2} \cos \frac{\sqrt{3}}{2} q_y \right). \tag{11}$$

Notice that Eq. (8) of Ref. 6 is identical to our Eq. (9) except that $A_{\mathbf{q}}^{13}$ and $A_{\mathbf{q}}^{31}$ are interchanged. The free energy of the model in harmonic approximation reads

$$F_2 = E_0 + \frac{1}{2} k_B T N \ln \left(\frac{12\pi J}{k_B T} \right) + \frac{1}{6} k_B T N \frac{3\sqrt{3}}{(2\pi)^2} \int_0^{2\pi/3} dq_x \int_0^{2\pi/\sqrt{3}} dq_y \ln(\det \mathbf{A_q}). \tag{12}$$

The free energy (12) is minimum for

$$\phi_1 = \phi_M = \pi, \quad \phi_2 = \phi_3 = \cos^{-1} \left(\frac{1+h}{2} \right) \tag{13}$$

when $0 \leq h \leq 1$ and

$$\phi_1 = \phi_M = \cos^{-1}\left(\frac{h^2-3}{2h}\right),$$
$$\phi_2 = \phi_3 = -\cos^{-1}\left(\frac{h^2+3}{4h}\right) \qquad (14)$$

when $1 \le h \le 3$.

A selection in the infinite ground-state manifold is performed by thermal fluctuations as correctly stated by Kawamura.[6] Incidentally, we notice that an imaginary free energy for $h > \sqrt{2}-1 = 0.414$ would be obtained on the basis of Ref. 6 because the determinant of $\mathbf{A_q}$ quoted there becomes negative at the zone boundary $\mathbf{q} = (2\pi/3, 2\pi/\sqrt{3})$ due to the discrepancy between our Eq. (9) and Eq. (8) of Ref. 6. However, the above discrepancy does not affect the ground-state configuration. The elementary excitation energies $\hbar\omega_{\mathbf{q}}^{(s)}$ are related to the eigenvalues of the $\mathbf{A_q}$ matrix given by Eq. (9) for $0 \le h \le 3$ or by Eq. (10) for $h > 3$. Indeed,

$$\hbar\omega_{\mathbf{q}}^{(s)} = 3J\lambda_{\mathbf{q}}^{(s)}, \quad s = 1,2,3, \qquad (15)$$

where $\lambda_{\mathbf{q}}^{(s)}$'s are the solutions of the equation

$$(1-\lambda_{\mathbf{q}})^3 - (1-\lambda_{\mathbf{q}})|\gamma_{\mathbf{q}}|^2 f(h) + g(h)\tfrac{1}{2}\left(\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3}\right) = 0 \qquad (16)$$

with

$$f(h) = \tfrac{1}{4}\left[(h+1)^4 - 2(h+1)^2 + 4\right],$$
$$g(h) = \tfrac{1}{4}(h+1)^2\left[(h+1)^2 - 2\right] \qquad (17)$$

for $0 \le h \le 1$ and

$$f(h) = 1 + \tfrac{1}{8}\left(h^2-5\right)^2, \quad g(h) = \tfrac{1}{8}\left(h^2-5\right) \qquad (18)$$

for $1 \le h \le 3$. For $h \ge 3$ the eigenvalues $\lambda_{\mathbf{q}}^{(s)}$'s are the solutions of the equation

$$(h-2-\lambda_{\mathbf{q}})^3 - 3(h-2-\lambda_{\mathbf{q}})|\gamma_{\mathbf{q}}|^2 + \left(\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3}\right) = 0. \qquad (19)$$

The elementary excitation energies in the (1,1) direction are shown for $h=0$, $h=0.5$, $h=1$ in Fig. 1, and for $h=2$, $h=3$, $h=4$ in Fig. 2, respectively. With our choice of axis the (1,1) direction corresponds to $0 < q_x < 2\pi/3$, $q_y = 0$. As one can see for $0 \le h \le 3$ no gap appears in the excitation spectrum, whereas a gap opens for $h > 3$. The absence of gap for $h \le 3$ is probably an artifact of the harmonic approximation because the lifting of the ground-state infinite degeneracy caused by the magnetic field at finite temperature suggests that a gap should appear if nonlinear contributions to the free energy were taken into account. We will return to this point in Sec. III.

In view of the promising experimental test by magnetic resonance in ABX_3 compounds[8] we give explicitly the field dependence of the uniform modes

$$\hbar\omega_0^{(1)} = 0, \quad \hbar\omega_0^{(2,3)} = \tfrac{3}{2}J\left[3 \mp (2h+h^2)\right] \qquad (20)$$

for $0 \le h \le 1$

$$\hbar\omega_0^{(1)} = 0, \quad \hbar\omega_0^{(2,3)} = \tfrac{3}{2}J\left[3 \mp \sqrt{1+\tfrac{1}{2}(h^2-5)^2}\right] \qquad (21)$$

for $1 \le h \le 3$

$$\hbar\omega_0^{(1,2)} = 3J(h-3), \quad \hbar\omega_0^{(3)} = 3Jh \qquad (22)$$

for $h > 3$.

Note that the qualitative behavior agrees with experimental data shown in Fig. 5b of Ref. 8. In contrast, a quite different behavior is found if the ground-state configuration was that assumed in Ref. 8 with a spin parallel to the field. In this case one should have

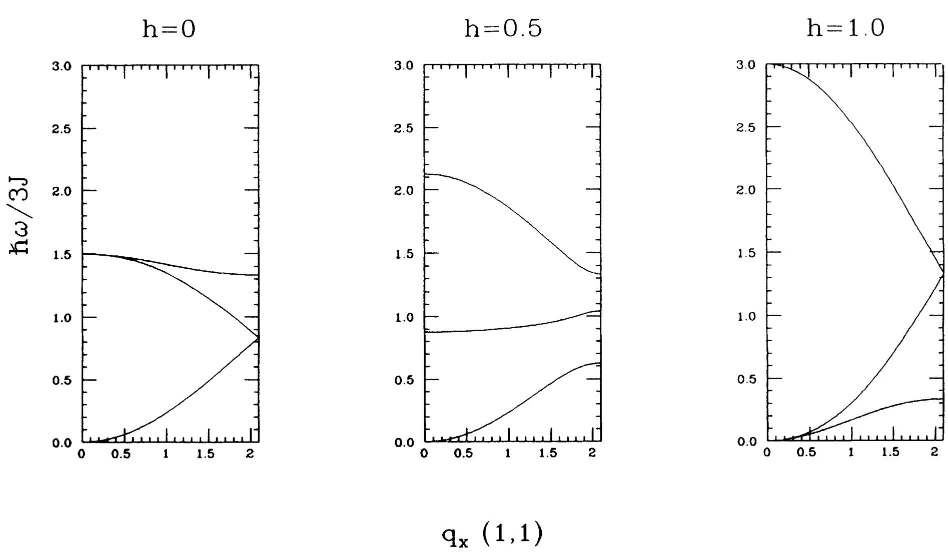

FIG. 1. Elementary excitation energies for $h=0$, 0.5, and 1 in harmonic approximation along the (1,1) direction.

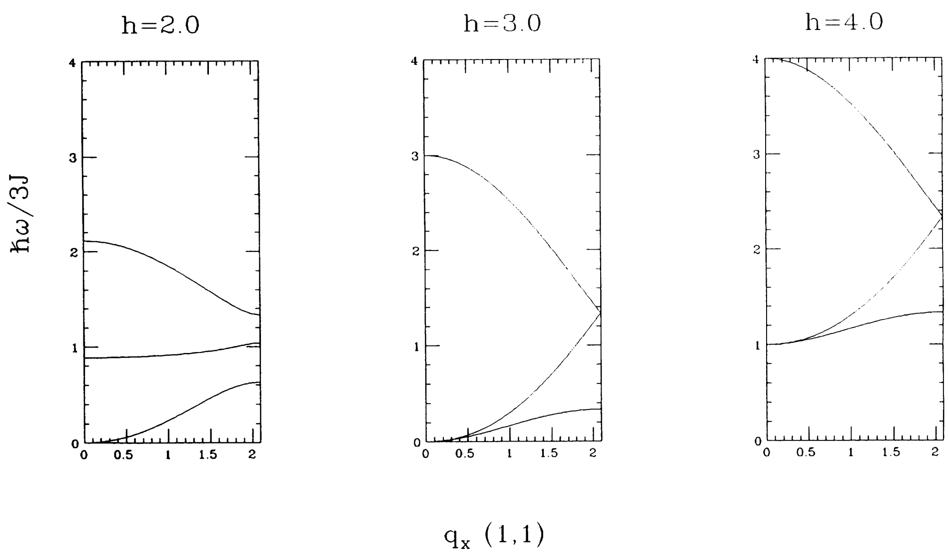

FIG. 2. Elementary excitation energies for $h = 2$, 3, and 4 in harmonic approximation along the (1,1) direction.

$$\hbar\omega_0^{(1)} = 0, \quad \hbar\omega_0^{(2,3)} = \tfrac{3}{2}J\left[3 \mp (2h - h^2)\right] \tag{23}$$

for $0 \le h \le 3$, so that a crossing between the gaps should occur at $h = 2$.

We consider now what happens at low but finite temperature in the neighborhood of $h = 1$. We are particularly interested in the mechanism that stabilizes the "up-up-down" phase over a finite region of the H-T plane as found by MC simulation.[4,5] If one limits oneself to linear approximation one should expect that such a configuration is stable only at $h = 1$ even for $T \neq 0$, because the corresponding free energy becomes imaginary when $h \neq 1$. Here we show that crucial nonlinear contributions to the thermal renormalization of the elementary excitations support LRO. Moreover, we find that the low-temperature phase boundaries between the configuration for $h \simeq 1$ and the low-field ($h < 1$) and the intermediate-field ($1 < h < 3$) configurations show the behavior suggested by the MC simulation.

A perturbative approach using $\mathcal{H}_2$ given by Eq. (7) as unperturbed Hamiltonian is prevented by divergences in T^2 contributions. For this reason we introduce a "trial" bilinear Hamiltonian where the coefficients $\tilde{A}_{\mathbf{q}}^{ss'}$ are variational parameters that is

$$\mathcal{H}_0 = 3J\sum_{s,s'=1}^{3}\sum_{\mathbf{q}}\psi_{-\mathbf{q}}^{(s)}\tilde{A}_{\mathbf{q}}^{ss'}\psi_{\mathbf{q}}^{(s')}. \tag{24}$$

So doing the perturbation expansion of the variational free energy reads

$$F_v = F_0 + \langle V + \mathcal{H}_2 - \mathcal{H}_0\rangle_0, \tag{25}$$

where F_0 is the free energy corresponding to the "trial" Hamiltonian $\mathcal{H}_0$

$$F_0 = E_0 + \frac{1}{2}k_BTN\ln\left(\frac{12\pi J}{k_BT}\right) + \frac{1}{2}k_BT\sum_{\mathbf{q}}\ln(\det\tilde{\mathbf{A}}_{\mathbf{q}}) \tag{26}$$

and $\langle\cdots\rangle_0$ means thermal average over the canonical ensemble of $\mathcal{H}_0$. The "effective" interaction potential V is

$$V = \mathcal{H}_4 - \frac{1}{2k_BT}\mathcal{H}_3^2, \tag{27}$$

where

$$\begin{aligned}\mathcal{H}_3 = -3J\sqrt{\frac{3}{N}}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}\delta_{\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3,0}\big[&\sin(\phi_1-\phi_2)(\gamma_{\mathbf{q}_3}\psi_{\mathbf{q}_1}^{(1)}\psi_{\mathbf{q}_2}^{(1)}\psi_{\mathbf{q}_3}^{(2)} - \gamma_{\mathbf{q}_1}^{*}\psi_{\mathbf{q}_1}^{(1)}\psi_{\mathbf{q}_2}^{(2)}\psi_{\mathbf{q}_3}^{(2)})\\ &+\sin(\phi_2-\phi_3)(\gamma_{\mathbf{q}_3}\psi_{\mathbf{q}_1}^{(2)}\psi_{\mathbf{q}_2}^{(2)}\psi_{\mathbf{q}_3}^{(3)} - \gamma_{\mathbf{q}_1}^{*}\psi_{\mathbf{q}_1}^{(2)}\psi_{\mathbf{q}_2}^{(3)}\psi_{\mathbf{q}_3}^{(3)})\\ &+\sin(\phi_3-\phi_1)(\gamma_{\mathbf{q}_3}\psi_{\mathbf{q}_1}^{(3)}\psi_{\mathbf{q}_2}^{(3)}\psi_{\mathbf{q}_3}^{(1)} - \gamma_{\mathbf{q}_1}^{*}\psi_{\mathbf{q}_1}^{(3)}\psi_{\mathbf{q}_2}^{(1)}\psi_{\mathbf{q}_3}^{(1)})\big].\end{aligned} \tag{28}$$

In Eq. (28) one has

$$\sin(\phi_1-\phi_2)=\sin(\phi_3-\phi_1)=\tfrac{1}{2}\sqrt{3-h^2-2h}\quad ,$$
$$\sin(\phi_2-\phi_3)=\tfrac{1}{2}(1+h)\sqrt{3-h^2-2h} \tag{29}$$

for $0 \le h \le 1$ and

$$\sin(\phi_1-\phi_2)=-\sin(\phi_3-\phi_1)=\tfrac{1}{4}\sqrt{10h^2-h^4-9},\quad \sin(\phi_2-\phi_3)=0 \tag{30}$$

for $1 \le h \le 3$. In Eq. (27) $\mathcal{H}_4$ reads

$$\begin{aligned}\mathcal{H}_4 = -\frac{3J}{4N}\sum_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_4}&\delta_{\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4,0}\\
\times\Bigg\{&\sum_{s=1}^{3}\psi^{(s)}_{\mathbf{q}_1}\psi^{(s)}_{\mathbf{q}_2}\psi^{(s)}_{\mathbf{q}_3}\psi^{(s)}_{\mathbf{q}_4}\\
&+\cos(\phi_1-\phi_2)\left[4\gamma_{\mathbf{q}_4}\psi^{(1)}_{\mathbf{q}_1}\psi^{(1)}_{\mathbf{q}_2}\psi^{(1)}_{\mathbf{q}_3}\psi^{(2)}_{\mathbf{q}_4}-6\gamma_{\mathbf{q}_3+\mathbf{q}_4}\psi^{(1)}_{\mathbf{q}_1}\psi^{(1)}_{\mathbf{q}_2}\psi^{(2)}_{\mathbf{q}_3}\psi^{(2)}_{\mathbf{q}_4}+4\gamma^*_{\mathbf{q}_1}\psi^{(1)}_{\mathbf{q}_1}\psi^{(2)}_{\mathbf{q}_2}\psi^{(2)}_{\mathbf{q}_3}\psi^{(2)}_{\mathbf{q}_4}\right]\\
&+\cos(\phi_2-\phi_3)\left[4\gamma_{\mathbf{q}_4}\psi^{(2)}_{\mathbf{q}_1}\psi^{(2)}_{\mathbf{q}_2}\psi^{(2)}_{\mathbf{q}_3}\psi^{(3)}_{\mathbf{q}_4}-6\gamma_{\mathbf{q}_3+\mathbf{q}_4}\psi^{(2)}_{\mathbf{q}_1}\psi^{(2)}_{\mathbf{q}_2}\psi^{(3)}_{\mathbf{q}_3}\psi^{(3)}_{\mathbf{q}_4}+4\gamma^*_{\mathbf{q}_1}\psi^{(2)}_{\mathbf{q}_1}\psi^{(3)}_{\mathbf{q}_2}\psi^{(3)}_{\mathbf{q}_3}\psi^{(3)}_{\mathbf{q}_4}\right]\\
&+\cos(\phi_3-\phi_1)\left[4\gamma_{\mathbf{q}_4}\psi^{(3)}_{\mathbf{q}_1}\psi^{(3)}_{\mathbf{q}_2}\psi^{(3)}_{\mathbf{q}_3}\psi^{(1)}_{\mathbf{q}_4}-6\gamma_{\mathbf{q}_3+\mathbf{q}_4}\psi^{(3)}_{\mathbf{q}_1}\psi^{(3)}_{\mathbf{q}_2}\psi^{(1)}_{\mathbf{q}_3}\psi^{(1)}_{\mathbf{q}_4}+4\gamma^*_{\mathbf{q}_1}\psi^{(3)}_{\mathbf{q}_1}\psi^{(1)}_{\mathbf{q}_2}\psi^{(1)}_{\mathbf{q}_3}\psi^{(1)}_{\mathbf{q}_4}\right]\Bigg\}.\end{aligned} \tag{31}$$

In Eq. (31) one has

$$\cos(\phi_1-\phi_2)=\cos(\phi_3-\phi_1)=-\frac{1+h}{2},$$
$$\cos(\phi_2-\phi_3)=\frac{h^2+2h-1}{2} \tag{32}$$

for $0 \le h \le 1$ and

$$\cos(\phi_1-\phi_2)=\cos(\phi_3-\phi_1)=\frac{h^2-5}{4},\quad \cos(\phi_2-\phi_3)=1 \tag{33}$$

for $1 \le h \le 3$. Minimization of F_v with respect to the variational parameters $\tilde{A}^{ss'}_{\mathbf{q}}$ leads to

$$\tilde{A}^{ss'}_{\mathbf{q}}=A^{ss'}_{\mathbf{q}}+\Sigma^{ss'}_{\mathbf{q}}. \tag{34}$$

For convenience of the reader we give explicitly the $\mathbf{A}_{\mathbf{q}}$ matrix for the three configurations that meet at the triple point $(h=1, T=0)$

$$\mathbf{A}^-_{\mathbf{q}}=\begin{pmatrix}1 & -\frac{1+h}{2}\gamma_{\mathbf{q}} & -\frac{1+h}{2}\gamma^*_{\mathbf{q}}\\ -\frac{1+h}{2}\gamma^*_{\mathbf{q}} & 1 & \frac{h^2+2h-1}{2}\gamma_{\mathbf{q}}\\ -\frac{1+h}{2}\gamma_{\mathbf{q}} & \frac{h^2+2h-1}{2}\gamma^*_{\mathbf{q}} & 1\end{pmatrix} \tag{35}$$

for $0 \le h \le 1$. In the "up-up-down" configuration one has

$$\mathbf{A}^0_{\mathbf{q}}=\begin{pmatrix}h & -\gamma_{\mathbf{q}} & -\gamma^*_{\mathbf{q}}\\ -\gamma^*_{\mathbf{q}} & h & \gamma_{\mathbf{q}}\\ -\gamma_{\mathbf{q}} & \gamma^*_{\mathbf{q}} & 2-h\end{pmatrix} \tag{36}$$

and

$$\mathbf{A}^+_{\mathbf{q}}=\begin{pmatrix}1 & \frac{h^2-5}{4}\gamma_{\mathbf{q}} & \frac{h^2-5}{4}\gamma^*_{\mathbf{q}}\\ \frac{h^2-5}{4}\gamma^*_{\mathbf{q}} & 1 & \gamma_{\mathbf{q}}\\ \frac{h^2-5}{4}\gamma_{\mathbf{q}} & \gamma^*_{\mathbf{q}} & 1\end{pmatrix} \tag{37}$$

for $1 \le h \le 3$. The "self-energy" $\Sigma^{ss'}_{\mathbf{q}}$ in Eq. (34) is given by

$$\langle V\psi^{(s)}_{-\mathbf{q}}\psi^{(s')}_{\mathbf{q}}\rangle^c_0=6J\sum_{r,r'=1}^{3}\langle\psi^{(s')}_{\mathbf{q}}\psi^{(r)}_{-\mathbf{q}}\rangle_0\Sigma^{rr'}_{\mathbf{q}}\langle\psi^{(r')}_{\mathbf{q}}\psi^{(s)}_{-\mathbf{q}}\rangle_0. \tag{38}$$

The superscript c means cumulant. In the neighborhood of $h=1$ we perform a low-temperature expansion in $|1-h|$ retaining only temperature-independent contributions linear in $|1-h|$ and temperature-dependent contributions independent of $|1-h|$. Within this approximation $\mathcal{H}_3$ can be neglected because it contains a $|1-h|^{1/2}$ factor so that its second-order contribution to the free energy [see Eq. (25)] is proportional to $|1-h|$ times a temperature-dependent factor vanishing for vanishing temperature, while $\mathcal{H}_4$ is accounted for because it provides temperature-dependent contributions of the same order as $\mathcal{H}_3$ but independent of $|1-h|$. The solution of Eq. (38) reads

$$\mathbf{\Sigma}_{\mathbf{q}}=\begin{pmatrix}-\Sigma_{11} & \Sigma_{12}\gamma_{\mathbf{q}} & \Sigma_{13}\gamma^*_{\mathbf{q}}\\ \Sigma_{12}\gamma^*_{\mathbf{q}} & -\Sigma_{22} & -\Sigma_{23}\gamma_{\mathbf{q}}\\ \Sigma_{13}\gamma_{\mathbf{q}} & -\Sigma_{23}\gamma^*_{\mathbf{q}} & -\Sigma_{22}\end{pmatrix}, \tag{39}$$

where

$$\Sigma_{11}=\tfrac{1}{6}t(3I_1-4I_2), \tag{40}$$

$$\Sigma_{12}=\tfrac{1}{3}t(I_1-I_2), \tag{41}$$

$$\Sigma_{22} = \tfrac{1}{6}t(I_1 - 4I_2), \qquad (42)$$

$$\Sigma_{23} = \tfrac{1}{3}t(I_1 + I_2), \qquad (43)$$

with $t = k_B T/2J$ and

$$I_1 = \frac{3}{N}\sum_{\mathbf{q}} \frac{1 - |\gamma_{\mathbf{q}}|^2}{\det \tilde{\mathbf{A}}_{\mathbf{q}}} \simeq -\frac{\sqrt{3}}{2\pi}\ln(tI_1), \qquad (44)$$

$$I_2 = \frac{3}{N}\sum_{\mathbf{q}} \frac{|\gamma_{\mathbf{q}}|^2 - \frac{1}{2}(\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3})}{\det \tilde{\mathbf{A}}_{\mathbf{q}}} \simeq \frac{1}{2}I_1. \qquad (45)$$

The approximate values of I_1 and I_2 are obtained by keeping the leading singular contribution. Notice that

$$\begin{aligned}\det \tilde{\mathbf{A}}_{\mathbf{q}} = {} & 1 - 3|\gamma_{\mathbf{q}}|^2 + (\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3}) \\ & -(\Sigma_{11} + 2\Sigma_{22})(1 - |\gamma_{\mathbf{q}}|^2) \\ & +2(2\Sigma_{12} + \Sigma_{23})\left[|\gamma_{\mathbf{q}}|^2 - \tfrac{1}{2}\left(\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3}\right)\right]. \end{aligned} \qquad (46)$$

In the long-wavelength limit we have

$$\begin{aligned}\det \tilde{\mathbf{A}}_{\mathbf{q}} & \simeq \frac{3}{16}q^4 + \frac{1}{12}q^2 t(I_1 + 10I_2) \\ & \simeq \frac{3}{16}q^4 + \frac{\sqrt{3}}{4\pi}q^2 t|\ln t| \end{aligned} \qquad (47)$$

As one can see the convergence of I_1 and I_2 is assured just by the singular temperature-dependent contribution in $\det \tilde{\mathbf{A}}_{\mathbf{q}}$, whereas a standard perturbation approach cannot pick up this contribution.

We are now able to compare the free energies of the three phases, which meet at the triple point $h = 1, t = 0$. Let us call ΔF^+ the difference between the free energies of the *high* field ($h > 1$) and the "up-up-down" phases and ΔF^- the difference between the free energies of the *low* field ($h < 1$) and the "up-up-down" phases. We obtain

$$\Delta F^+ = -JN(h-1)^2 - \tfrac{1}{6}k_B TN(h-1) \qquad (48)$$

and

$$\Delta F^- = -JN(1-h^2) + \tfrac{1}{6}k_B TN(1-h)G, \qquad (49)$$

where

$$G = \frac{3}{N}\sum_{\mathbf{q}} \frac{1 + 5|\gamma_{\mathbf{q}}|^2 - 3(\gamma_{\mathbf{q}}^3 + \gamma_{\mathbf{q}}^{*3})}{\det \tilde{\mathbf{A}}_{\mathbf{q}}} \simeq \frac{2\sqrt{3}}{\pi}|\ln t|. \qquad (50)$$

The above approximate value of G is obtained by keeping the leading singular contribution. In our approximation we find that the "up-up-down" phase is stable in the H-T plane below $h = 1$ and above the line of equation

$$h = 1 - \frac{2}{\pi\sqrt{3}}t|\ln t|. \qquad (51)$$

In the low-temperature limit our evaluation of the phase boundary is in good agreement with the extrapolation of the MC data. For example, for $t = 0.1$ both Eq. (51) and MC simulation give $h \simeq 0.9$.

III. ORDER PARAMETER

The interesting MC simulations[4,5] are suitably interpreted on the basis of the order parameters

$$\langle\psi_{\parallel}\rangle = \frac{1}{3}\left(\langle\cos\phi_1\rangle + e^{2i\pi/3}\langle\cos\phi_2\rangle + e^{4i\pi/3}\langle\cos\phi_3\rangle\right),$$

$$\langle\psi_{\perp}\rangle = -\frac{1}{3}\left(\langle\sin\phi_1\rangle + e^{2i\pi/3}\langle\sin\phi_2\rangle + e^{4i\pi/3}\langle\sin\phi_3\rangle\right). \qquad (52)$$

In Fig. 3 of Ref. 4 are quoted the magnitudes of these order parameters as function of the magnetic field at fixed temperature. The spin configuration suggested in Fig. 2 of the same reference is rotated by 180° with respect to the configuration suggested by the analytic expansion.[6,7] However, we show that the spin configuration consistent with Fig. 3 of Ref. 4 is just that obtained in Refs. 6 and 7. Indeed, we have evaluated the *zero-temperature* values of $|\langle\psi_{\parallel}\rangle|$ and $|\langle\psi_{\perp}\rangle|$, obtaining

$$\begin{aligned}|\langle\psi_{\parallel}\rangle| &= \frac{1}{3}\left[\left(\frac{3}{2}\cos\phi - \frac{1}{2}h\right)^2 + \frac{3}{4}\sin^2\phi\left(\frac{3 - h^2 + 2h\cos\phi}{1 + h^2 - 2h\cos\phi}\right)\right]^{1/2}, \\ |\langle\psi_{\perp}\rangle| &= \frac{1}{3}\left[\frac{9}{4}\sin^2\phi + \frac{3}{4}(h - \cos\phi)^2\left(\frac{3 - h^2 + 2h\cos\phi}{1 + h^2 - 2h\cos\phi}\right)\right]^{1/2}. \end{aligned} \qquad (53)$$

In Figs. 3 and 4 we draw $|\langle\psi_{\parallel}\rangle|$ and $|\langle\psi_{\perp}\rangle|$ for $\phi = 0$ (the configuration suggested by Ref. 4) and for $\phi = \phi_M$ [the configuration suggested by Eqs. (13) and (14)]. It is clearly seen that the order parameters obtained by the MC simulations[4] are a natural evolution of the zero-temperature order parameters corresponding to $\phi = \phi_M$.

We have performed MC simulation on a sample of 18 × 18, 24 × 24, and 30 × 30 spins for temperatures lower than those explored in Ref. 4. We find that our results for $t = 0.1$ shown in Fig. 4 agree with the zero-temperature values of the order parameters and have the same qualitative behavior as the $t = 0.4$ values of Ref. 4.

We would like to remark on the existence of LRO phases in this model. The proof of existence of LRO could be hardly achieved on the basis of MC simulation even for the largest samples considered in Refs. 4 and 5. Indeed we prove that LRO is absent in a triangular planar antiferromagnet, even if a magnetic field is present, when we limit ourselves to the harmonic approximation. Indeed let us consider the average component of the spins on a generic sublattice

$$\langle\cos(\phi_s + \psi_i^{(s)})\rangle = \cos\phi_s\langle\cos\psi_i^{(s)}\rangle, \qquad (54)$$

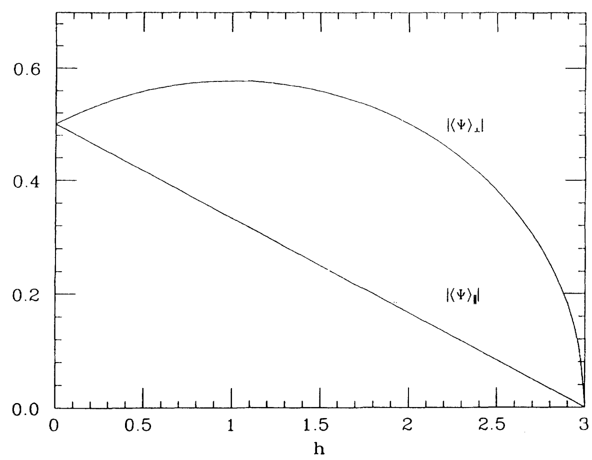

FIG. 3. Zero-temperature order parameters $|\langle\psi_\parallel\rangle|$ and $|\langle\psi_\perp\rangle|$ for $\phi = 0$ as function of h.

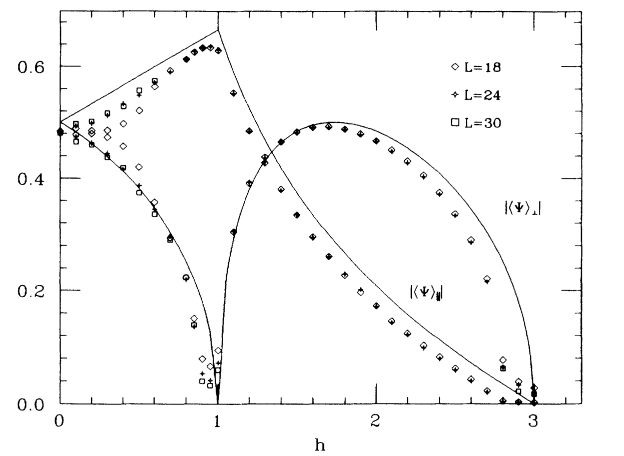

FIG. 4. Zero-temperature order parameters $|\langle\psi_\parallel\rangle|$ and $|\langle\psi_\perp\rangle|$ for $\phi = \phi_M$ as function of h are shown by continuous curves. Diamonds, stars, and squares are the same quantities at $t = 0.1$ obtained by MC simulation for 18×18, 24×24, and 30×30 samples, respectively.

where

$$\langle\cos\psi_i^{(s)}\rangle = 1 - \frac{1}{2!}\langle\left(\psi_i^{(s)}\right)^2\rangle + \frac{1}{4!}\langle\left(\psi_i^{(s)}\right)^4\rangle - \frac{1}{6!}\langle\left(\psi_i^{(s)}\right)^6\rangle + \cdots . \quad (55)$$

Notice that

$$\langle\left(\psi_i^{(s)}\right)^2\rangle = \frac{t}{3}\frac{1}{N/3}\sum_{\mathbf{q}}\left(\mathbf{A}_{\mathbf{q}}^{-1}\right)_{ss}, \quad (56)$$

where $\mathbf{A}_{\mathbf{q}}^{-1}$ is the inverse of the matrix $\mathbf{A}_{\mathbf{q}}$ defined in Eqs. (9) and (10). The series (55) can be summed to give

$$\langle\cos\psi_i^{(s)}\rangle = \exp\left(-\frac{t}{6}\frac{3\sqrt{3}}{(2\pi)^2}\int_0^{2\pi/3}dq_x\int_0^{2\pi/\sqrt{3}}dq_y\left(\mathbf{A}_{\mathbf{q}}^{-1}\right)_{ss}\right). \quad (57)$$

The explicit expression of $(\mathbf{A}_{\mathbf{q}}^{-1})_{ss}$ for the first sublattice with $0 < h < 1$ reads

$$\left(\mathbf{A}_{\mathbf{q}}^{-1}\right)_{11} = \frac{1 - \frac{1}{4}\left(h^2+2h-1\right)^2 + \frac{1}{8}q^2\left(h^2+2h-1\right)^2 + \cdots}{\frac{1}{16}q^2\left[9 - h^2(h+2)^2\right] - \frac{1}{256}q^4\left[33 - 9h^2(h+2)^2\right] + \cdots}. \quad (58)$$

As one can see $\langle\cos\psi_i^{(s)}\rangle$ vanishes at any finite temperature even if the magnetic field is present because of a logarithmic divergence in the argument of the exponential. However, this divergence for a sample of linear size L should give

$$\langle\cos(\phi_s + \psi_i^{(s)})\rangle = \cos\phi_s(L)^{-(\sqrt{3}/12\pi)t}. \quad (59)$$

At $t = 0.4$ for $L = 24$ and $L = 48$ one obtains $0.943\cos\phi_s$ and $0.931\cos\phi_s$, respectively. This apparent LRO is clearly an artifact of the finite size of the sample at least when only harmonic contributions are taken into account. Note that the harmonic approximation provides very accurate values of the internal energy for temperatures as high as $t = 0.1$, as we have checked by comparison between the low-temperature expansion and MC calculation for selected values of the magnetic field. Obviously we do not exclude that nonlinear contributions could support LRO. Indeed we expect that nonlinear contributions modify crucially Eq. (57). Consequently the spin average is modified, and the LRO described by Eq. (59), which is an artifact of the finite size in the harmonic approximation, becomes reliable via a possible replacement of the "unphysical" power of L by a nonlinear contribution, say a power of T. Further theoretical effort will be necessary to clarify this point. However, we can prove that a genuine LRO is supported by anharmonic contributions for the "up-up-down" phase. On the basis of the calculations performed in Sec. II we have to replace $(\mathbf{A}_{\mathbf{q}}^{-1})_{ss}$ by $(\tilde{\mathbf{A}}_{\mathbf{q}}^{-1})_{ss}$ in Eq. (57). For $h = 1$ we have

$$\langle\cos(\phi_s + \psi_i^{(s)})\rangle = \cos\phi_s e^{-(\sqrt{3}/12\pi)t|\ln t|} = t^{+0.046t}\cos\phi_s. \quad (60)$$

In Sec. II we have seen that linear approximation for $0 \le h \le 3$ provides at least one excitation with zero energy cost at the zone center (see Figs. 1 and 2) and we have anticipated that this should be an artifact of the harmonic approximation. We give partial support to this guess on the basis of our evaluation of the leading nonlinear contributions for $h = 1$. We find the following values of the uniform mode energies in the "up-up-down" configuration.

$$\hbar\tilde{\omega}_0^{(1)} = 0, \quad \hbar\tilde{\omega}_0^{(2)} = 12J\Sigma, \quad \hbar\tilde{\omega}_0^{(3)} = 9J(1-\Sigma), \qquad (61)$$

where

$$\Sigma \simeq \frac{\sqrt{3}}{12\pi} t|\ln t| \qquad (62)$$

We notice that linear approximation provides two zero-energy uniform modes at $h = 1$, while nonlinear effects we have accounted for lift one of them. It is reasonable to think that higher-order nonlinear contributions lift even the last zero-energy uniform mode.

On the basis of the analytic dependence on t shown in Eq. (60) one expects a significant thermal demagnetization in the low-temperature limit, but this peculiar behavior is restricted to a very narrow range of temperature because of the smallness of the numerical coefficient appearing in the exponential. An analogous scenario was recently found[9] on the ferro-helix phase boundary of the quantum Heisenberg tetragonal model with in-plane interactions up to third neighbors and a ferromagnetic nearest-neighbor interplane interaction. In this model the linear spin-wave theory suggests a divergent demagnetization at any finite temperature, whereas crucial nonlinear contributions to the spin-wave self-energy restoring LRO appear already at the first-order Hartree-Fock correction. The resulting LRO shows in this model a peculiar behavior in the low-temperature range because the *order by thermal disorder*[10] becomes effective only at intermediate temperatures, so that a steep demagnetization of 40% or 50% sets up within temperature $t = 0.1$ or 0.2.[9]

Finally, we offer a comment on the persistence of the $\sqrt{3}\times\sqrt{3}$ periodicity in an external magnetic field at finite temperature. A simple argument has been given in the Appendix of Ref. 5 showing that the ground state ($T = 0$ configuration) consists of the spin arrangement where in each triangle

$$\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 - \frac{\mu\mathbf{H}}{6J} = \mathbf{0}. \qquad (63)$$

At finite but low temperature ($\beta \to \infty$), a straightforward saddle-point evaluation of the partition function can show that such configurations must dominate the thermodynamics. However, the locking of commensurate helices by an external magnetic field at nonzero T can be rigorously proven, because δ-like terms appear in an exact low-temperature low-field expansion of the free energy.[11] In particular such contribution for 120° three-sublattice configuration reads

$$\Delta F_3 = -\tfrac{1}{6}(\mu H)^3 A_1 N k_B T \cos(3\phi) \sum_{\mathbf{G}} \delta(3\mathbf{Q} - \mathbf{G}), \qquad (64)$$

where $\mathbf{G}$ is a reciprocal lattice wave vector and $\mathbf{Q}$ is the helix wave vector $(4\pi/3, 0)$:

$$A_1 = -\frac{9}{2}\left(\frac{1}{9J}\right)^3 I(\mathbf{Q}), \qquad (65)$$

where

$$I(\mathbf{Q}) = \frac{1}{N}\sum_{\mathbf{q}} \frac{[J(\mathbf{Q}+\mathbf{q}) - J(\mathbf{q})][J(\mathbf{Q}-\mathbf{q}) - J(\mathbf{q})]}{[2J(\mathbf{Q}) - J(\mathbf{Q}+\mathbf{q}) - J(\mathbf{q})][2J(\mathbf{Q}) - J(\mathbf{Q}-\mathbf{q}) - J(\mathbf{q})]} \qquad (66)$$

with

$$J(\mathbf{q}) = 2J\left(\cos q_x + 2\cos\frac{1}{2}q_x \cos\frac{\sqrt{3}}{2}q_y\right). \qquad (67)$$

By numerical integration we have $I(\mathbf{Q}) = 0.1524$. Substituting this value in the free energy (64) we obtain

$$\Delta F_3 = \tfrac{1}{6}k_B T N h^3 0.2032 \cos(3\phi) \sum_{\mathbf{G}} \delta(3\mathbf{Q} - \mathbf{G}), \qquad (68)$$

which coincides with the expansion of Eq. (12) for small fields except for the δ factor. Equation (68) shows that the $\sqrt{3}\times\sqrt{3}$ periodicity is preserved at finite temperature as a special case of the more general locking of commensurate helices. In the present situation the helical structure is caused by the misfit between antiferromagnetism and triangular lattice (frustration from lattice topology). However, a generic helix can be produced on a generic lattice by suitable exchange competitions (frustration from competition).

IV. SUMMARY AND CONCLUDING REMARKS

We have shown that analytic expansion[6,7] and MC simulations[4,5] give concordant suggestions about the phase diagram in the field-temperature (H-T) plane. To this end we have also performed MC calculations at temperature low enough to match with the zero-temperature analytic result. We have explicitly evaluated the elementary excitation energies obtained in harmonic approximation and we have found that no gap appears for vanishing wave vectors in the ordered phases although thermal fluctuations select one spin configuration out of the zero-temperature infinitely degenerate manifold. We believe, however, that nonlinear contributions should provide a gap at finite temperature. This is a relevant point because the model should be disordered at any finite temperature if the essential physics was fully treated within the harmonic approximation. Further theoretical effort is required to understand whether the LRO suggested by MC calculation is a reliable result or it is an artifact of the finite-size sample. However we have proven that a genuine LRO onsets at $h = 1$ in the "up-up-down" phase. The mechanism supporting LRO originates from crucial nonlinear effects that we have accounted for by a variational approach because they cannot be treated conveniently by a standard perturbation approach owing to divergences in T^2 contributions. Such crucial nonlinear contributions lead also to the stability over a finite region of the H-T plane of the "up-up-down" configuration. The persistence of the $\sqrt{3} \times \sqrt{3}$ periodicity in an external magnetic field is traced back to the locking of commensurate helix configurations in an external magnetic field.[11]

Finally, we suggest $CsVX_3$,with X=Cl, Br, I (Ref. 12) as possible candidates to see the phenomenology of the triangular planar antiferromagnet in an external magnetic field. From a magnetic point of view these systems are chains along the c axis of localized spins $S = 3/2$. The chains are arranged to form triangular lattice in the planes perpendicular to the c axis. The small easy-plane anisotropy forces the system in the symmetry class of the present model. As concerns the transition in the H-T plane we are interested in, the relevant coupling is the interchain coupling $J' \simeq 10^{-3}$ meV (Ref. 12) so that the saturation field $h_c = 3$ in our notation corresponds to external magnetic fields of 1.4, 4.4, and 18.8 kG, for $CsVCl_3$, $CsVBr_3$, and $CsVI_3$, respectively. Magnetic resonances in $CsCuCl_3$,[8] where the weak interacting spin chains with $S = 1/2$ can be simulated at temperature low enough as a triangular Heisenberg antiferromagnet with easy plane anisotropy, show that the uniform modes are changed by an external magnetic field perpendicular to the chains in a way confirming the lifting of infinite degeneracy of the minimum energy configurations, as suggested by the low-temperature free-energy expansion of the TPA model.

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