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Quantum fluctuations and ground state of weakly interacting helix spin chains in a magnetic field

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Abstract. Ferromagnetic spin chains of a hexagonal lattice coupled by a weak antiferromagnetic interaction J_1 develop a helix arrangement if the intrachain antiferromagnetic NNN exchange J_2 is sufficiently large. We show that the classical minimum energy spin configuration is an *umbrella* when an external magnetic field is applied. The scenario is dramatically changed by quantum fluctuations. Indeed we find that the zero point motion forces the spins in a plane containing the magnetic field so that classical expectation is deceptive for our model. Our result is obtained by controlled expansion in the low field-long wavelength modulation limit.

PACS. 75.10.Jm Quantized spin models – 75.30.Ds Spin waves – 75.50.-y Studies of specific magnetic materials

1 Introduction

Hexagonal spin chains weakly interacting *via* NN antiferromagnetic exchange interaction J_1 forming a hexagonal lattice are a suitable model in order to describe the magnetic properties of the ABX_3 compounds, where A is an alkali element, B a magnetic ion, and X a halogen [1]. A peculiar example is $CsCuCl_3$ [2] where the NN intrachain interaction J_0 is ferromagnetic and a Dzyaloshinsky-Morija interaction forces the spins in the basal planes and causes a long period spin modulation along the c-axis. This compound was extensively investigated both theoretically [3–5] and experimentally [2,6–10]. Indeed this compound shows an interesting phenomenology when an external magnetic field parallel or perpendicular to the c-axis is applied. Magnetic resonance [2] and magnetization [7] as function of the external magnetic field were measured and satisfactorily explained theoretically [3–5]. The magnetic resonance data were shown to be relied to the lifting by quantum fluctuations of the classical infinite degeneracy of the triangular antiferromagnetic model when an in-plane external magnetic field is applied [3,11–13]. The plateau or the jump in the uniform magnetization [7] induced by a field perpendicular or parallel to the c-axis were ascribed to quantum fluctuations which cause a reorientation of the spins [3–5].

Even though experimental data are well understood on the basis of in-plane spin configurations [8,10] deeply affected by quantum fluctuations a still open point is the possible onset of out-of-plane spin patterns when a high external magnetic field ($H \simeq 0.5H_s$, where H_s is the saturation field) is applied perpendicular to the chain [14]. In reference [14] out-of-plane spin configurations are found *via* numerical evaluation of the minimum energy spin configuration of a classical spin model suitable for $CsCuCl_3$. An effective biquadratic exchange coupling is also proposed to mimic quantum fluctuations.

Since analytic study of possible out-of-plane spin configurations is not possible for the Hamiltonian model suitable for $CsCuCl_3$, we consider an isotropic spin model supporting the zero field configuration characterized by the $(\frac{1}{3}, \frac{1}{3}, q)$ order wave vector. We do not expect our results to be conclusive in order to prove or disprove the onset of an out-of-plane spin configurations in $CsCuCl_3$. Anyway, the scenario we study is of the same kind as that observed in $CsCuCl_3$, at least from a qualitative point of view, so that we hope to cast a glance at the behavior of the actual compound.

In order to separate the mechanism responsible of the spin modulation along the chain from that forcing the spins to rotate in the basal plane (these two mechanisms are intrinsecally connected in the Dzyaloshinsky-Morija interaction [14]), we consider NN and NNN intrachain competing isotropic exchange interactions that lead to a long period helix along the chain, even though they do not select any plane of rotation for the spins. Note that we do not introduce any mechanism favoring the in-plane spin configuration.

In classical approximation (Sect. 2) we find that an *umbrella* (U) configuration (where spins are spiralling on the surface of a cone having the axis parallel to the field) is stable with respect to a planar (P) configuration (where spins lie in a plane containing the magnetic field). Note that this is a consequence of the helix along the c-axis, whereas in absence of this modulation the umbrella and

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infinite in-plane spin configurations have the same classical energy [3,12,15]. Anyway the plane of the spins in the P phase is selected only if some anisotropy is introduced. In Section 3 we evaluate the leading contribution of the zero point motion energy as an expansion of the magnetic field. We find that the classical scenario is overturned and the U configuration is replaced by a P configuration supported by quantum fluctuations. Finally, summary and conclusions are contained in Section 4.

2 "Classical" ground state

We consider a hexagonal lattice of ferromagnetic chains coupled by weak antiferromagnetic interaction. We assume the external magnetic field directed along a line of in-plane NN (x-axis). The Hamiltonian we consider reads

$$\mathcal{H} = -J_0 \sum_{n\boldsymbol{\delta}_z} \mathbf{S}_n \cdot \mathbf{S}_{n+\boldsymbol{\delta}_z} - J_2 \sum_{n\boldsymbol{\delta}'_z} \mathbf{S}_i \cdot \mathbf{S}_{n+\boldsymbol{\delta}'_z} + J_1 \sum_{i\boldsymbol{\delta}} \mathbf{S}_i \cdot \mathbf{S}_{i+\boldsymbol{\delta}} - g\mu_B \mathbf{H} \cdot \sum_i \mathbf{S}_i \tag{2.1}$$

where $2J_0$ and $2J_2$ are the NN and NNN intrachain competing exchange interactions, $2J_1$ is the in-plane antiferromagnetic exchange interaction, $\mathbf{H}$ is the external magnetic field, g is the Landé factor, μ_B is the Bohr magneton, n labels the spins along the ferromagnetic chains, i labels the sites of each one of the three sublattices in which the hexagonal lattice is divided. Vectors $\boldsymbol{\delta}_z = (0,0,\pm c)$, $\boldsymbol{\delta}'_z = (0,0,\pm 2c)$ join a spin with its intrachain NN and NNN, respectively; $\boldsymbol{\delta} = (a,0,0)$, $(-\frac{1}{2}a, \pm\frac{\sqrt{3}}{2}a, 0)$ join a spin with its in-plane NN.

Strictly following the approach of reference [5] we consider a long period spin modulation along the c-axis in order to perform the continuum approximation. As for P configurations the energy of the model becomes

$$\mathcal{H} = 2J_0 N S^2 \left[-1 - \frac{J_2}{J_0} + \frac{1}{L}\int_0^L \mathcal{E}(z) dz \right] \tag{2.2}$$

where

$$\begin{aligned}\mathcal{E}(z) = \frac{1}{6}\sum_{j=1}^{3} \Bigg\{ & c^2\left(1+4\frac{J_2}{J_0}\right)\left(\frac{d\phi_j}{dz}\right)^2 \\ - & \frac{c^4}{12}\left(1+16\frac{J_2}{J_0}\right)\left[\left(\frac{d\phi_j}{dz}\right)^4 + \left(\frac{d^2\phi_j}{dz^2}\right)^2\right] \\ + & \frac{c^6}{360}\left(1+64\frac{J_2}{J_0}\right)\left[\left(\frac{d\phi_j}{dz}\right)^6 + 9\left(\frac{d\phi_j}{dz}\right)^2\left(\frac{d^2\phi_j}{dz^2}\right)^2 \right. \\ + & \left.\left(\frac{d^3\phi_j}{dz^3}\right)^2 - 2\left(\frac{d\phi_j}{dz}\right)^3\left(\frac{d^3\phi_j}{dz^3}\right)\right]\Bigg\} \\ + & \frac{J_1}{J_0}\Bigg\{\cos(\phi_1(z)-\phi_2(z)) + \cos(\phi_2(z) \\ - & \phi_3(z)) + \cos(\phi_3(z)-\phi_1(z)) \\ - & h\Big[\cos(\phi_1(z)) + \cos(\phi_2(z)) + \cos(\phi_3(z))\Big]\Bigg\}\end{aligned} \tag{2.3}$$

with $h = g\mu_B H/6J_1 S$; $\phi_1(z)$, $\phi_2(z)$, $\phi_3(z)$ are the angles between the spins of the three sublattices and the external magnetic field, respectively. Note that the continuum expansion in reference [5] was limited to the first order whereas an expansion up to third order is required in our model to get significant results. The minimum energy configuration is obtained by solving the Euler-Lagrange equations. The first equation reads

$$\begin{aligned}\frac{1}{3}\Bigg\{ & c^2\left(1+4\frac{J_2}{J_0}\right)\frac{d^2\phi_1}{dz^2} - \frac{c^4}{2}\left(1+16\frac{J_2}{J_0}\right) \\ \times & \left(\frac{d\phi_1}{dz}\right)^2\left(\frac{d^2\phi_j}{dz^2}\right) \\ + & \frac{c^6}{120}\left(1+64\frac{J_2}{J_0}\right)\left[5\left(\frac{d\phi_1}{dz}\right)^4\right. \\ \times & \left(\frac{d^2\phi_1}{dz^2}\right) + 3\left(\frac{d^2\phi_1}{dz^2}\right)^3 \\ + & \left. 4\left(\frac{d\phi_1}{dz}\right)\left(\frac{d^2\phi_1}{dz^2}\right)\left(\frac{d^3\phi_1}{dz^3}\right) - \left(\frac{d\phi_1}{dz}\right)^2\left(\frac{d^4\phi_1}{dz^4}\right)\right]\Bigg\} \\ + & \frac{J_1}{J_0}\Big[\sin(\phi_1(z)-\phi_2(z)) \\ + & \sin(\phi_1(z)-\phi_3(z)) - h\sin(\phi_1(z))\Big] = 0.\end{aligned} \tag{2.4}$$

The other two Euler-Lagrange equations are obtained by cyclic permutation of sublattice labels.

For $h = 0$ the solution is an incommensurate regular helix given by

$$\phi_j(z) = \phi_j + q_0 z \tag{2.5}$$

where $\phi_1 = \phi$, $\phi_2 = \phi - \frac{2\pi}{3}$, $\phi_3 = \phi + \frac{2\pi}{3}$. The energy density reads

$$\mathcal{E}(z) = \frac{1}{2}\left[(cq_0)^2\left(1+4\frac{J_2}{J_0}\right) - \frac{1}{12}(cq_0)^4\left(1+16\frac{J_2}{J_0}\right) + \frac{1}{360}(cq_0)^6\left(1+64\frac{J_2}{J_0}\right)\right] - \frac{3J_1}{2J_0}\cdot \tag{2.6}$$

Minimization of the energy leads to the helix wave vector in the continuum approximation

$$(cq_0)^2 = 8\epsilon\left(1 - \frac{10}{3}\epsilon\right) + O(\epsilon^3) \tag{2.7}$$

where $\epsilon = -(\frac{1}{4} + \frac{J_2}{J_0}) > 0$. Note that the exact helix wave vector is [16]

$$\cos(cq_0) = \frac{1}{1+4\epsilon} \tag{2.8}$$

that agrees to the approximate solution (2.7) within $O(\epsilon^3)$.

For $h \neq 0$ we look for solutions like

$$\begin{aligned}\phi_j(z) = \phi_j + qz + a_1 h \sin(qz+\phi_j) \\ + a_2 h^2 \sin(2(qz+\phi_j)) + ...\end{aligned} \tag{2.9}$$

for $j = 1, 2, 3$. Substitution of the series solution (2.9) in (2.4) leads to

$$a_1 = \frac{-\frac{2}{3}}{1 + \frac{128 J_0}{9 J_1}\epsilon^2\left(1 - \frac{19}{3}\epsilon\right)} \tag{2.10}$$

$$a_2 = -\frac{1}{3}a_1 \frac{1 + \frac{9}{4}a_1\left[1 + \frac{256 J_0}{9 J_1}\epsilon^2\left(1 - \frac{22}{3}\epsilon\right)\right]}{1 + \frac{512 J_0}{9 J_1}\epsilon^2\left(1 - \frac{28}{3}\epsilon\right)} \tag{2.11}$$

and

$$\begin{aligned}\mathcal{E}(z) = \frac{1}{2}\Bigg[&(cq)^2\left(1 + 4\frac{J_2}{J_0}\right)\left(1 + \frac{1}{2}a_1^2 h^2\right)\\ &- \frac{1}{12}(cq)^4\left(1 + 16\frac{J_2}{J_0}\right)\left(1 + \frac{7}{2}a_1^2 h^2\right)\\ &+ \frac{1}{360}(cq)^6\left(1 + 64\frac{J_2}{J_0}\right)\left(1 + \frac{31}{2}a_1^2 h^2\right)\Bigg]\\ &- \frac{3J_1}{2J_0} + \frac{3J_1}{2J_0}a_1\left(1 + \frac{3}{4}a_1\right)h^2. \end{aligned} \tag{2.12}$$

Minimization with respet to q leads to the magnetic field dependence of the helix wave vector. We obtain

$$(cq)^2 = (cq_0)^2 - 24\epsilon\left(1 - \frac{28}{3}\epsilon\right)a_1^2 h^2 \tag{2.13}$$

with cq_0 given by (2.7). The minimun energy is

$$\begin{aligned}E_0^{(P)} = 2J_0 N S^2\Bigg[&-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0} - 8\epsilon^2(1 - 4\epsilon) - \frac{J_1}{2J_0}h^2\\ &+ \frac{80}{9}\epsilon^2\left(1 - \frac{44}{5}\epsilon\right)h^2 - \frac{4096 J_0}{27 J_1}\epsilon^4 h^2\Bigg].\end{aligned} \tag{2.14}$$

We stress that all non vanishing h dependent contributions for vanishing ϵ are taken into account in equation (2.14) [3]. Note that infinite planar spin configurations have the same energy (2.14). Indeed $E_0^{(P)}$ is independent of ϕ the arbitrary phase of the first sublattice (see Eqs. (2.9, 2.5)).

The classical energy of the umbrella configuration is

$$\begin{aligned}E_0^{(U)} = 2J_0 N S^2\Bigg\{&-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0} - \frac{8\epsilon^2}{1 + 4\epsilon} - \frac{J_1}{2J_0}h^2\\ &+ \frac{8\epsilon^2}{9(1 + 4\epsilon)}\left[1 + \frac{J_0}{J_1}\frac{16\epsilon^2}{9(1 + 4\epsilon)}\right]^{-2}h^2\\ &+ \frac{J_0}{J_1}\frac{128\epsilon^4}{81(1 + 4\epsilon)^2}\left[1 + \frac{J_0}{J_1}\frac{16\epsilon^2}{9(1 + 4\epsilon)}\right]^{-2}h^2\Bigg\}\end{aligned} \tag{2.15}$$

where the spiral wave vector is given by

$$cq = \cos^{-1}\left(\frac{1}{1 + 4\epsilon}\right) \tag{2.16}$$

and the apex cone angle is

$$\theta = \cos^{-1}\frac{\frac{h}{3}}{1 + \frac{J_0}{J_1}\frac{16\epsilon^2}{9(1 + 4\epsilon)}}\cdot \tag{2.17}$$

In the limit of long period modulation ($\epsilon \to 0$) the energy of the U phase becomes

$$\begin{aligned}E_0^{(U)} = 2J_0 N S^2\Bigg[&-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0} - 8\epsilon^2(1 - 4\epsilon) - \frac{J_1}{2J_0}h^2\\ &+ \frac{8}{9}\epsilon^2(1 - 4\epsilon)h^2 - \frac{128 J_0}{81 J_1}\epsilon^4 h^2\Bigg].\end{aligned} \tag{2.18}$$

As one can see the P phase is unstable with respect to the U phase when a spiral along the c axis is present. Indeed $[E_0^{(U)} - E_0^{(P)}]/2J_0 N S^2 \simeq -8\epsilon^2 h^2$.

3 Zero point motion energy

In order to get the leading zero point motion contribution we have worked out the spin wave analysis of the model (2.1). Such analysis is the direct generalization of our previous results obtained for a 3D hexagonal antiferromagnet [3]. The bilinear Hamiltonian obtained from equation (2.1) by the standard spin-boson transformation is the same as equation (A.6) of reference [3] with $\eta = \eta_0 = 0$, provided that a term $4J_2 S(1 - \cos(2cq_z))$ is added in the curl brakets of the first term. We may perform analytic calculations only for $J_2/J_0 > -1/4$ otherwise the spin wave excitations in the P configuration become unstable. The extreme value that assures collinear configurations along the c axis is $\epsilon = 0$. In evaluating the zero point motion contribution we assume $\epsilon = 0$ since the long period modulation along c axis is expected to lead to vanishing contributions for vanishing ϵ. For $J_2/J_0 > -1/4$ one has

$$\begin{aligned}\Delta E_0^{(P)} &= 2J_0 N S\left(-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0}\right) + \frac{1}{2}\sum_{s=1}^{3}\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}^{s}\\ &= 2J_0 N S\Bigg(-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0}\\ &\quad + \frac{1}{3\pi^3}\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} dx dy dz \sum_{s=1}^{3}\sqrt{\lambda_s}\Bigg)\end{aligned} \tag{3.1}$$

where λ_s are the roots of the cubic equation

$$\lambda^3 - a\lambda^2 + b\lambda - c = 0 \tag{3.2}$$

with

$$\begin{aligned}a = 3&\left[1 - \cos z + \frac{J_2}{J_0}(1 - \cos(2z)) + \frac{3J_1}{2J_0}\right]^2\\ &+ 2\left(\frac{3J_1}{2J_0}\right)^2 s_1|\gamma|^2\end{aligned} \tag{3.3}$$

$$
\begin{aligned}
b = & \left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]^2 \\
& \times\left\{3\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]^2\right. \\
& \left. - s_2\left(\frac{3J_1}{2J_0}\right)^2|\gamma|^2\right\}+\left(\frac{3J_1}{2J_0}\right)^2 \\
& \times\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right] \\
& \times\left\{2s_1\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]|\gamma|^2\right. \\
& \left. +\frac{3J_1}{4J_0}\big(s_2-s_1^2\big)\big(\gamma^3+\gamma^{*3}\big)\right\} \\
& -\left(\frac{3J_1}{2J_0}\right)^2\left\{3\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)\right.\right. \\
& \left.+\frac{3J_1}{2J_0}\right]^2|\gamma|^2+\frac{3J_1}{2J_0}s_1\left[1-\cos z\right. \\
& \left.+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]\big(\gamma^3+\gamma^{*3}\big) \\
& \left.-\left(\frac{3J_1}{2J_0}s_1\right)^2|\gamma|^4\right\}
\end{aligned}
\tag{3.4}
$$

$$
\begin{aligned}
c = & \left\{\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]^3\right. \\
& -s_2\left(\frac{3J_1}{2J_0}\right)^2\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]|\gamma|^2 \\
& \left.+\frac{1}{2}(s_2-1)\left(\frac{3J_1}{2J_0}\right)^3\big(\gamma^3+\gamma^{*3}\big)\right\} \\
& \times\left\{\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]^3\right. \\
& -3\left(\frac{3J_1}{2J_0}\right)^2\left[1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0}\right]|\gamma|^2 \\
& \left.+\left(\frac{3J_1}{2J_0}\right)^3\big(\gamma^3+\gamma^{*3}\big)\right\}
\end{aligned}
\tag{3.5}
$$

where

$$
s_1=-\frac{3}{2}+\frac{1}{2}h^2\,,\quad s_2=\frac{3}{4}+\frac{1}{4}h^2\rho(h,\phi) \tag{3.6}
$$

$$
\gamma=\frac{1}{3}\big(e^{i\frac{2x}{3}}+2e^{-i\frac{x}{3}}\cos y\big) \tag{3.7}
$$

$$
\rho(h,\phi)= \frac{4-4h\cos\phi(4\cos^2\phi-1)+h^2(16\cos^2\phi-3)-6h^3\cos\phi+h^4}{1-2h\cos\phi+h^2}\,. \tag{3.8}
$$

Note the dependence of a, b, c and, consequently, of λ_s, on ϕ. This is because the zero point motion lifts the infinite degeneracy of the classical energy. The zero point motion for the U phase is

$$
\begin{aligned}
\Delta E_0^{(U)} &= 2J_0NS\left(-\frac{3J_1}{2J_0}-1-\frac{J_2}{J_0}\right)+\frac{1}{2}\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}} \\
&= 2J_0NS\left(-\frac{3J_1}{2J_0}-1-\frac{J_2}{J_0}+\frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dxdydz\sqrt{sd}\right)
\end{aligned}
\tag{3.9}
$$

where

$$
\begin{aligned}
s = & 1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big)+\frac{3J_1}{2J_0} \\
& +\frac{J_1}{J_0}\left(1-\frac{h^2}{6}\right)\Big(2\cos x\cos(2y)+\cos(2x)\Big)
\end{aligned}
\tag{3.10}
$$

$$
\begin{aligned}
d = & 1-\cos z+\frac{J_2}{J_0}\big(1-\cos(2z)\big) \\
& +\frac{3J_1}{2J_0}\left[1-\frac{1}{3}\Big(2\cos x\cos(2y)+\cos(2x)\Big)\right].
\end{aligned}
\tag{3.11}
$$

The leading contributions in the zero point motion responsible of the stabilization of the P phase with respect to the U phase are proportional to h^2 [13,17] so we neglect terms of order $h^2 o(\epsilon)$. In particular, for $J_2/J_0=-1/4$ and low field one obtains

$$
\begin{aligned}
\Delta E_0^{(P)} = 2J_0NS\Big[& -\frac{3J_1}{2J_0}-\frac{3}{4}+c_0^{(P)}+c_2^{(P)}h^2 \\
& +c_3^{(P)}h^3\cos(3\phi)+O(h^4)\Big]
\end{aligned}
\tag{3.12}
$$

where

$$
c_0^{(P)}=\frac{1}{3\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dxdydz\sum_{s=1}^{3}\sqrt{\lambda_s} \tag{3.13}
$$

$$
c_2^{(P)}=\frac{1}{6\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dxdydz\sum_{s=1}^{3}\frac{\mu_s}{\sqrt{\lambda_s}} \tag{3.14}
$$

$$
c_3^{(P)}=\frac{1}{6\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dxdydz\sum_{s=1}^{3}\frac{\sigma_s}{\sqrt{\lambda_s}} \tag{3.15}
$$

with

$$
\begin{aligned}
\lambda_1 = & \left[\frac{1}{2}\big(1-\cos z\big)^2+\frac{3J_1}{2J_0}\big(1+2a_q\big)\right] \\
& \times\left[\frac{1}{2}\big(1-\cos z\big)^2+\frac{3J_1}{2J_0}\big(1-a_q\big)\right]
\end{aligned}
\tag{3.16}
$$

$$
\begin{aligned}
\lambda_2 = & \left[\frac{1}{2}\big(1-\cos z\big)^2+\frac{3J_1}{2J_0}\big(1+\frac{1}{2}a_q+\frac{\sqrt{3}}{2}b_q\big)\right] \\
& \times\left[\frac{1}{2}\big(1-\cos z\big)^2-\frac{3J_1}{2J_0}\big(1-a_q-\sqrt{3}b_q\big)\right]
\end{aligned}
\tag{3.17}
$$

$$\lambda_3 = \left[\frac{1}{2}(1-\cos z)^2 + \frac{3J_1}{2J_0}(1+\frac{1}{2}a_q - \frac{\sqrt{3}}{2}b_q)\right] \times \left[\frac{1}{2}(1-\cos z)^2 - \frac{3J_1}{2J_0}(1-a_q+\sqrt{3}b_q)\right] \quad (3.18)$$

$$a_q = \frac{1}{3}\Big(\cos\frac{2x}{3} + 2\cos y\cos\frac{x}{3}\Big)$$
$$b_q = \frac{2}{3}\sin\frac{x}{3}\Big(\cos\frac{x}{3} - \cos y\Big) \quad (3.19)$$

$$\mu_s = \left(\frac{3J_1}{2J_0}\right)^2\Bigg\{(a_q^2+b_q^2)\lambda_s^2 + \frac{3}{2}\left(\frac{3J_1}{2J_0}\right)^3\Bigg[\left(\frac{3J_1}{2J_0}\right)(a_q^2+b_q^2)^2 - \left(\frac{1}{2}(1-\cos z)^2 + \frac{3J_1}{2J_0}\right)a_q(a_q^2-3b_q^2)\Bigg]\lambda_s - \Bigg[\left(\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right)(a_q^2+b_q^2) - \frac{3J_1}{2J_0}a_q(a_q^2-3b_q^2)\Bigg] \times \Bigg[\left(\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right)^3 - 3\left(\frac{3J_1}{2J_0}\right)^2 - \left(\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right)(a_q^2+b_q^2) + 2\left(\frac{3J_1}{2J_0}\right)^2 a_q(a_q^2-3b_q^2)\Bigg]\Bigg\} \times \left(3\lambda_s^2 - 2a_0\lambda_s + b_0\right)^{-1} \quad (3.20)$$

$$\sigma_s = \left(\frac{3J_1}{2J_0}\right)^2\Bigg\{\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]^3 - 3\left(\frac{3J_1}{2J_0}\right)^2\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right](a_q^2+b_q^2) + 2\left(\frac{3J_1}{2J_0}\right)^3 a_q(a_q^2-3b_q^2) - \left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]\lambda_s\Bigg\} \times \Bigg\{\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right](a_q^2+b_q^2) - \frac{3J_1}{2J_0}a_q(a_q^2-3b_q^2)\Bigg\}\left(3\lambda_s^2 - 2a_0\lambda_s + b_0\right)^{-1} \quad (3.21)$$

with

$$a_0 = 3\Bigg\{\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]^2 - \left(\frac{3J_1}{2J_0}\right)^2(a_q^2+b_q^2)\Bigg\} \quad (3.22)$$

$$b_0 = 3\Bigg\{\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]^4 - \frac{9}{4}\left(\frac{3J_1}{2J_0}\right)^2\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]^2(a_q^2+b_q^2) + \frac{1}{2}\left(\frac{3J_1}{2J_0}\right)^3\left[\frac{1}{2}(1-\cos z)^2+\frac{3J_1}{2J_0}\right]a_q(a_q^2-3b_q^2) + \frac{3}{4}\left(\frac{3J_1}{2J_0}\right)^4(a_q^2+b_q^2)^2\Bigg\}. \quad (3.23)$$

Numerical evaluation of integrals appearing in equations (3.13–3.15) for $J_1/J_0 = 0.175$, a value appropriate to $CsCuCl_3$, gives

$$\varDelta E_0^{(P)} = 2J_0NS\big[-0.025155 + 0.248h^2 + 0.237h^3\cos(3\phi) + O(h^4)\big]. \quad (3.24)$$

For the U phase one has

$$\varDelta E_0^{(U)} = 2J_0NS\left[-\frac{3J_1}{2J_0} - \frac{3}{4} + c_0^{(U)} + c_2^{(U)}h^2 + O(h^4)\right] \quad (3.25)$$

where

$$c_0^{(U)} = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi dxdydz\sqrt{sd} \quad (3.26)$$

$$c_2^{(U)} = -\frac{1}{18\pi^3}\left(\frac{3J_1}{2J_0}\right)\int_0^\pi\int_0^\pi\int_0^\pi dxdydz \times(2\cos x\cos y + \cos 2x)\sqrt{d/s} \quad (3.27)$$

$$s = \frac{1}{2}(1-\cos z)^2 + \frac{3J_1}{2J_0}\left[1+\frac{2}{3}(2\cos x\cos y+\cos 2x)\right] \quad (3.28)$$

$$d = \frac{1}{2}(1-\cos z)^2 + \frac{3J_1}{2J_0}\left[1-\frac{1}{3}(2\cos x\cos y+\cos 2x)\right]. \quad (3.29)$$

Numerical evaluation gives $c_0^{(U)} = c_0^{(P)} = 0.987345$ as expected since it is the magnetic field that selects between P and U phases [13,17]. So we have

$$\varDelta E_0^{(U)} = 2J_0NS\big[-0.025155 + 0.65h^2 + O(h^4)\big]. \quad (3.30)$$

The difference between the energy of the U and P phase is

$$\varDelta E = E^{(U)} - E^{(P)} = 2J_0NS^2 \times\left[-8\epsilon^2\left(1-\frac{28}{3}\epsilon\right)h^2 + \frac{12160}{81}\frac{J_0}{J_1}\epsilon^4h^2 + \frac{0.40}{S}h^2\right]. \quad (3.31)$$

Extrapolation of equation (3.31) shows that P-phase is stable with respect to U-phase for $\epsilon < \sqrt{\frac{0.40}{8S}}$. For instance, $(cq_0) \simeq \frac{\pi}{2}$ for $S = 1/2$ and $(cq_0) \simeq 0.88$ for $S = 5/2$. This means that the P phase is always stable for helices characterized by a long period wave vector. We recall that $\epsilon \simeq 10^{-3}$ is required to have the helix pitch observed in $CsCuCl_3$.

In order to test the stability of the commensurate planar phase, characterized by a helix wave vector $(\frac{1}{3},\frac{1}{3},0)$ in r.l.u., with respect to the incommensurate umbrella phase for any applied field we evaluate the U phase energy by

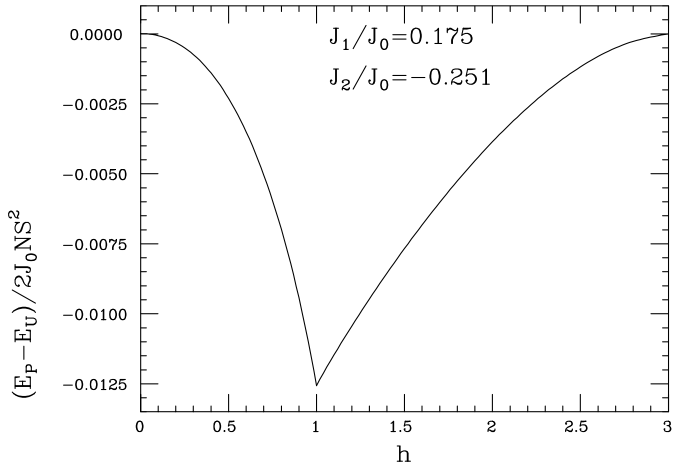

Fig. 1. The difference between the energy of the incommensurate umbrella phase and the commensurate planar phase *versus* magnetic field for parameters suitable for $CsCuCl_3$

means of equations (2.15, 3.9) valid for any field. We compare this energy with that obtained for the commensurate P phase

$$E^{(P)}\left(\frac{1}{3},\frac{1}{3},0\right) = 2J_0NS^2\left[-\frac{3J_1}{2J_0} - 1 - \frac{J_2}{J_0} - \frac{J_1}{2J_0}h^2\right] + \Delta E_0^P \quad (3.32)$$

where $\Delta E_0^{(P)}$ is given by equation (3.1). The difference between the energies of the U (incommensurate) phase and the P (commensurate) phase is shown in Figure 1 *versus* field form zero to saturation field. The commensurate P phase is stable over the whole range of the applied magnetic fields except for a very narrow region close to the origin. Indeed at $h = 0$ the incommensurate U phase is stable, as expected, because $\Delta E = [E^{(P)}(\frac{1}{3},\frac{1}{3},0) - E_0^{(U)}]/2J_0NS^2 = \frac{8\epsilon^2}{1+4\epsilon} \simeq 8\times10^{-6}$. However, at $h \simeq \sqrt{20S}\epsilon$ the commensurate P phase becomes stable and it remains stable to the saturation field.

So we conclude that the incommensurate U phase is replaced by a suitable planar phase for *any* magnetic field. Indeed equation (3.31) proves that an incommensurate P phase is the minimum energy configuration in the low field limit where analytic description of the incommensurate P phase is possible. Moreover the commensurate P phase is stable with respect to the incommensurate U phase for non vanishing values of h.

A fortiori the out-of-plane U phase should be excluded if some planar anisotropy would be present. Anyway the spins are forced in a plane containing the magnetic field by quantum fluctuations and planar anisotropy only chooses the c plane. We stress that the out-of-plane phase is ruled out by quantum fluctuations even though any easy-plane anisotropy term is absent. On the contrary out-of-plane spin configurations are obtained in [14] where both DM interaction and easy-plane exchange anisotropies are present. This is not surprising if one neglects quantum fluctuations because the applied magnetic field favors umbrella like configurations so that a sufficiently high magnetic field may overcome the effect of the anisotropic terms, if they are not too large. Indeed the out-of-plane configuration is drastically reduced and finally suppressed by an increasing exchange anisotropy [14]. On the other hand we think that the effective biquadratic exchange assumed to mimic quantum fluctuations [14] could be a poor approximation of quantum effects. Indeed the biquadratic term does not change substantially the classical scenario. This poor treatment of quantum fluctuations could be the origin of the surviving of the out-of-plane configuration found in reference [14]. In particular, we have tested the above phenomenological treatment of quantum fluctuations by an analytical series expansion of the ground state in powers of the field for the 2D triangular antiferromagnet (TAF). We find that the difference between the energies of umbrella and planar configurations for the expansion at low field of the zero point motion [17] is

$$\Delta E = 2J_1NS^2\left[\frac{0.082}{2S}h^2 + \frac{0.039}{2S}h^3 + ...\right] \quad (3.33)$$

to be compared with the same differnce obtained expanding the phenomenological ground state (13) of reference [14]

$$\Delta E = 2J_1NS^2\left[\frac{3J_2}{4J_1}h^2 - \frac{J_2}{2J_1}h^3 + ...\right]. \quad (3.34)$$

Note that J_2 in (3.34) is the strength of the biquadratic exchange. As one can see the quadratic term in h^2 may be recovered assuming $J_2 = 0.055J_1/S$ but the coefficient of h^3 has an opposit sign in equations (3.33, 3.34). This casts some doubt about the reliability of the phenomenological treatment of quantum fluctuations [14].

4 Summary and conclusions

We have investigated the possibility of out-of-plane spin configurations containing the external magnetic field perpendicular to the c axis of a hexagonal lattice of spin chains weakly coupled by an antiferromagnetic exchange interaction J_1. The intrachain NN J_0 and NNN J_2 interactions are ferro- and antiferromagnetic, respectively. We consider values of $J_2/J_0 \lesssim -1/4$ so assuring a long period spin modulation along the c axis. In Section 2 we evaluate the classical energy of the umbrella (U) phase and a planar (P) phase. We find that the U phase is stable with respect to infinite degenerate P configurations. Note that U and P phases have the same energy when no modulation along the c axis is present [3]. In Section 3 we evaluate the zero point motion energy at the leading order in $1/S$. The classical scenario is overturned by quantum fluctuations and P configuration is stabilized. We have obtained these results by a controlled expansion for low magnetic field and long period modulation.

However, we expect that the stability of the P phase is assured even for high values of the magnetic field. Indeed the energy of a commensurate three sublattice configuration characterized by a wave vector $(\frac{1}{3}, \frac{1}{3}, 0)$ in r.l.u. is certainly higher than the energy of the true P configuration. Notwithstanding we find that even such a rough treatment of the energy of the P phase is lower than the energy of the U phase easy to evaluate for any field. So we conclude that quantum fluctuations stabilize the P phase not only at low field but also at high field. We are not able to localize the possible incommensurate-commensurate (IC-C) field induced phase transition between planar configurations since we are able to give a controlled description of the IC phase only at low fields. Note that we have neglected any easy-plane anisotropy favoring the c planes. Such anisotropy is often present in ABX_3 compounds and in particular in $CsCuCl_3$ where the mechanism producing the long period spin modulation and part of the easy-plane anisotropy originates from the Dzyaloshinsky-Morija interaction. The incommensurate helix observed in this compound is characterized by the wave vector $(\frac{1}{3}, \frac{1}{3}, 0.014)$ [6]. On the basis of our analysis where easy-plane anisotropy is not considered we think that quantum fluctuations play a crucial role in forcing the spins into a plane containing the applied magnetic field. This could be the reason because the experimental data of $CsCuCl_3$ are satisfactorily described in classical approximation disregarding the out-of-plane spin configuration [5].

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