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LETTER TO THE EDITOR

Characterisation of the quantum helix in Heisenberg models

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Abstract. Unexpected features in helimagnets are produced by quantum fluctuations. On hexagonal and tetragonal lattices with competing in-plane interactions up to third-nearest neighbours, the zero-temperature phase diagram, obtained in the classical approximation, is strongly affected by quantum effects in the neighbourhood of the triple point where ferromagnetic, antiferromagnetic, and helical phases coexist. The ferromagnetic configuration turns out to be unstable against long-wavelength quantum fluctuations, allowing a novel helix of quantum origin to have its onset and the corresponding ferro–helix phase transition to become first order. This result has been obtained by an exact evaluation of the ground-state energy within Q^4 contributions. However, the value of the helix wavevector Q cannot be obtained by such a calculation. Here we give this wavevector as a function of the Hamiltonian parameters by evaluating at leading order in $1/S$ the Q^6 contributions to the ground-state energy. Our result is consistent with the assumption that the quantum helix wavevector is small.

Competing exchange interactions in Heisenberg models are able to produce helimagnetic configurations [1]. The traditional approach to obtaining the phase diagram in parameter space neglects quantum fluctuations entirely [2]. Only recently have efforts been made to understand their role, and new interesting features have been found in tetragonal and hexagonal Heisenberg models with in-plane competing interactions up to third neighbours. The phase diagram of a classical Heisenberg model on a simple hexagonal lattice is shown in figure 1.

A T-matrix evaluation of the ground-state energy, exact within Q^4 contributions, where Q is the helix wavevector, has been performed along the ferro–helix phase boundary [3]. The F–H phase transition, continuous in the classical approximation, is shifted and becomes first order near the F–AF–H triple point. This calculation proves that the ferromagnetic configuration can be unstable with respect to long-wavelength helical modulations supported by quantum effects. This approach goes well beyond previous treatments based on an evaluation of the zero-point-motion energy at leading order in $1/S$ with the classical approximation as the starting point [4].

Anyway, it is interesting that reliable indications from a qualitative and semiquantitative point of view of the onset of the new quantum helix can be obtained by truncation of the T-matrix expansion of the ground-state energy at leading order in $1/S$; the values of the parameters at which the transition becomes first order differ from the exact ones by less than ten per cent for $J' = 0$ and $S = 1$. For this reason we think that the ordering in $1/S$ is a tool that is as reliable for studying non-collinear configurations as it is for

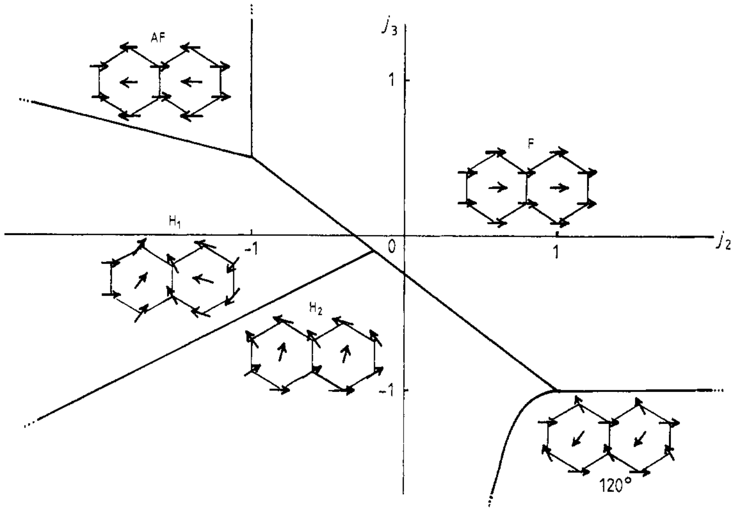

Figure 1. The phase diagram of the classical Heisenberg model on a simple hexagonal lattice at zero temperature taken from [5]. F, AF, H_1, H_2 and 120° indicate ferromagnetic, antiferromagnetic, two helical, and the 120°–three-sublattice phase, respectively.

studying the collinear ones, if the value of the helix wavevector is evaluated by minimising the ground-state energy only after having taken quantum contributions into account.

Insurmountable difficulties are introduced if one takes the classical stage as the starting point, because in this case the helix wavevector is fixed from the beginning, so quantum effects produce spin-wave frequencies that are not well defined [4].

Here we avoid the aforementioned difficulties by going to the order Q^6 in the evaluation of the contributions to the ground-state energy at leading order in $1/S$ and treating the helix wavevector $\boldsymbol{Q}$ as a variational parameter to be determined only after having accounted for the quantum contributions we are interested in.

The Hamiltonian of our model reads

$$H = -\sum_{\alpha=1}^{3} J_\alpha \sum_{i,\delta_\alpha} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta_\alpha} - J' \sum_{i,\delta'} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta'} \qquad (1)$$

where i labels the sites on a hexagonal lattice, and $\boldsymbol{\delta}_\alpha$ and $\boldsymbol{\delta}'$ are vectors joining site i to its in-plane neighbours of the αth shell and to its out-of-plane nearest neighbours, respectively. J_1 is positive, while the other exchange couplings can have either sign.

The customary steps in treating modulated spin patterns are the introduction of a local quantisation axis [5] spiralling in the plane according to a helix of wavevector $\boldsymbol{Q}$, and the realisation of the spin operators in terms of bose creation and annihilation operators through the well known Dyson–Maleev transformation [6].

We are interested in long-wavelength modulations up to order Q^6, so the reduced ground-state energy of our model at leading order in $1/S$, evaluated on the classical F–H transition line $1 + 3j_2 + 4j_3 = 0$, reads

$$e_G = E_G/4J_1 S^2 N = e_{cl} + \Delta/S \qquad (2)$$

where

$$e_{\rm cl} = -\tfrac{3}{4} - \tfrac{1}{4}j_2 - \tfrac{1}{3}j' + \tfrac{3}{64}(1+j_2)(aQ_x)^4 - \tfrac{3}{512}(1+j_2)(aQ_x)^6 \tag{3}$$

with $j_\alpha = J_\alpha/J_1$, and a the in-plane lattice constant. Here we refer to a helical modulation whose wavevector lies along an in-plane next-nearest-neighbours row ($Q_y = 0$), because we are interested in the neighbourhood of the F-AF-H triple point where the helix configuration is the $\rm H_1$ configuration [5]. Δ is the long-wavelength contribution to the zero-point-motion energy:

$$\Delta = -\tfrac{1}{32}I_0(aQ_x)^4 - \tfrac{1}{128}I_1(aQ_x)^6 \tag{4}$$

where

$$I_0 = \frac{1}{4\pi^2}\int_0^\pi\int_0^\pi {\rm d}x\,{\rm d}y\, b^2(x,y)D(x,y) \tag{5}$$

$$I_1 = \frac{1}{8\pi^2}\int_0^\pi\int_0^\pi {\rm d}x\,{\rm d}y\, b(x,y)D(x,y)[D(x,y)^2(\varepsilon(x,y)+j'/3)\alpha(x,y)b(x,y) - c(x,y)] \tag{6}$$

with

$$b(x,y) = \cos x\cos y + j_2(\cos x\cos 3y + 2\cos 2x) + 4j_3\cos 2x\cos y \tag{7}$$

$$\alpha(x,y) = 2 - \cos x\cos y + j_2(6 - 2\cos 2x - \cos x\cos 3y) + 4j_3(2-\cos 2x\cos 2y) \tag{8}$$

$$c(x,y) = \cos x\cos y + j_2(\cos x\cos 3y + 8\cos 2x) + 16j_3\cos 2x\cos 2y \tag{9}$$

$$\varepsilon(x,y) = 1 - \tfrac{1}{3}(\cos 2y + 2\cos x\cos y) + j_2[1 - \tfrac{1}{3}(\cos 2x + 2\cos x\cos 3y)] + j_3[1-\tfrac{1}{3}(\cos 4y + 2\cos 2x\cos 2y)] \tag{10}$$

$$D(x,y) = [\varepsilon(x,y)(\varepsilon(x,y) + \tfrac{2}{3}j')]^{-1/2}. \tag{11}$$

Equation (11) results from integration over the z coordinate. Equation (2) can be ordered in powers of Q as follows:

$$e_{\rm G} = e_0 + e_4Q_x^4 + e_6Q_x^6. \tag{12}$$

The possible minimum of $e_{\rm G}$ corresponds to

$$Q_x = (-2e_4/3e_6)^{1/2}. \tag{13}$$

It has been proved [3] by a calculation to *all orders* in $1/S$ that the Q^4 contribution becomes negative in the neighbourhood of the F-AF-H triple point, so the $\rm H_1$ helix overflows beyond the classical F-H boundary, driven by quantum fluctuations. This calculation is consistent under the hypothesis that the wavevector of the quantum helix is small. An indirect argument in favour of this assumption was provided by the comparison of the quantum helix ground-state energy with the antiferromagnetic ground-state energy at leading order in $1/S$ and the stability of the quantum helix with respect to the antiferromagnetic configuration was confirmed [7] for any $S > 1$.

In any case, a direct calculation of the value of $\boldsymbol{Q}$ was lacking. Here we deal with this omission by numerically computing $e_{\rm G}$ of (12) along the F-H classical transition line. The

Table 1. Coefficients of Q^4 and Q^6 in the reduced-energy expansion and values of Q of the quantum helix on the classical F–H$_1$ phase boundary ($j_2 = -(1 + 4j_3)/3$) are given for $S = 1$, $j' = 0.1$, and selected values of j_3.

j_3	e_4	e_6	Q
0.25	−0.0042	0.0145	0.441
0.30	−0.0131	0.0229	0.618
0.35	−0.0248	0.0389	0.652
0.40	−0.0416	0.0752	0.607
0.45	−0.0717	0.1980	0.491

Table 2. As table 1, but for $S = 1$ and $j' = 1$.

j_3	e_4	e_6	Q
0.30	−0.0038	0.0107	0.487
0.35	−0.0117	0.0176	0.666
0.40	−0.0216	0.0313	0.678
0.45	−0.0361	0.0711	0.582

results are shown in table 1 for $S = 1$ and $j' = 0.1$ and in table 2 for $S = 1$ and $j' = 1$. As can be seen, e_6 is positive—granted that the ground-state energy is minimised by a well defined wavevector $\boldsymbol{Q}$. Notice that the classical contribution to e_6 is negative. This is analogous to what happens to the coefficient of Q^4 where the classical and the quantum contributions have opposite signs: in both cases quantum effects are dominant in the neighbourhood of the F–AF–H triple point.

In the last column of each table we quote the values of Q for selected values of j_3 and for $S = 1$, $j' = 0.1$ (table 1) and $j' = 1$ (table 2). As can be seen, the resulting Q is small enough to give support to the approach recently elaborated in order to account for quantum fluctuations in helimagnets. The non-monotonous behaviour of the latter values is not to be treated as very significant because at the corresponding values of j_3 the antiferromagnetic phase takes over and the expansion in Q^6 becomes meaningless.

In summary, we report here a direct method for evaluating the wavevector of the quantum helix in the neighbourhood of the F–AF–H triple point of a hexagonal helimagnet. The existence of this quantum helix was proved on the basis of an evaluation of the ground-state energy *exact* to Q^4 by a T-matrix resummation of all Q^4 contributions. Notice that a T-matrix computation at higher order in Q is definitely of no value. However, it was found that a substantial quantum effect is already present in the contribution at leading order in $1/S$. On the basis of this observation we have evaluated the contribution to the ground-state energy up to Q^6 at leading order in $1/S$, so we are now able to compute the *value* of Q for the *quantum helix*.

We think that the present approach should be useful for investigating quantum effects in other regions of the phase diagram, namely in the neighbourhood of the H$_1$–H$_2$ transition line, which in the classical approximation is an *infinite degeneration line*, in the sense that an infinite number of inequivalent helices minimise the classical energy of the model [9]. We have already proved that suitable additional interactions can transform [10] this infinite degeneration line into a wedge-shaped intermediate phase where the helix wavevector explores all directions. A similar effect could be introduced by quantum fluctuations and we hope that this problem can be studied using an approach similar to that presented here.

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