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1989 J. Phys.: Condens. Matter 1 5151

(http://iopscience.iop.org/0953-8984/1/31/013)

J. Phys.: Condens. Matter 1 (1989) 5151–5155. Printed in the UK

Novel helix phase in the Heisenberg tetragonal model

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Received 3 August 1988

Abstract. The phase diagram of a classical tetragonal Heisenberg model with in-plane nearest, second-nearest, and third-nearest neighbour exchange interactions consists of ferromagnetic (F), antiferromagnetic (AF), and two helix (H1 and H2) configurations. The H1–H2 transition line is an infinite degeneration line, because infinite inequivalent helices minimise the energy of the model. A fourth-nearest neighbour interaction lifts the infinite degeneracy and makes the H1–H2 transition first order. In the hexagonal lattice a more complex interaction scheme, involving fifth- and sixth-nearest neighbours, supports a novel phase, in which the helix wavevector changes continuously spanning all directions. In the tetragonal lattice we find an analogous phase supported by a fifth-nearest neighbour interaction.

Renewed attention has recently been paid to classical models, even if one cannot exclude the possibility that quantum effects could dramatically affect the classical picture. Very interesting phenomena were discovered in classical magnetic models, such as soliton excitation (e.g. see [1]) and Kosterlitz–Thouless phase transition [2].

Concerning Heisenberg helimagnets, unorthodox configurations, which we call *degenerate helix* (DH), were found as the result of a suitable in-plane exchange competition in hexagonal and tetragonal models with interactions up to third-nearest neighbours J_1, J_2, and J_3 (3N model), assuming that the nearest neighbour (NN) interaction J_1 is ferromagnetic [3]. In figure 1 we give the phase diagram at zero temperature of the 3N classical Heisenberg model. Along the line $J_2 = 2J_3$, which we call the *degeneration line*, the energy of the 3N model is minimised by infinite inequivalent helices corresponding to infinite helix wavevectors $\boldsymbol{Q}$ satisfying the following equation:

$$\cos(aQ_x) + \cos(aQ_y) = -J_1/2J_2. \tag{1}$$

In the absence of any anisotropy the magnon spectrum vanishes for all $\boldsymbol{k} = \boldsymbol{Q}$ given by equation (1), leading to a catastrophic number of thermally excited spin deviations which destroy long range order (LRO) even in 3D at any finite temperature. An analogous scenario was found in the rhombohedral Heisenberg antiferromagnet (RAF model) [4] with NN interactions, because the in-plane interaction favours the 120° three sublattice configuration, whereas the interplane interaction prefers collinear configurations so that frustration is produced and a DH scenario is established.

An interesting question regards the survival of the DH scenario in the presence of additional perturbations as, for instance, further interactions. It is well established that a fourth-nearest neighbour interaction [5] removes the infinite degeneracy in the 3N model and makes the H1–H2 transition first order in both tetragonal and hexagonal

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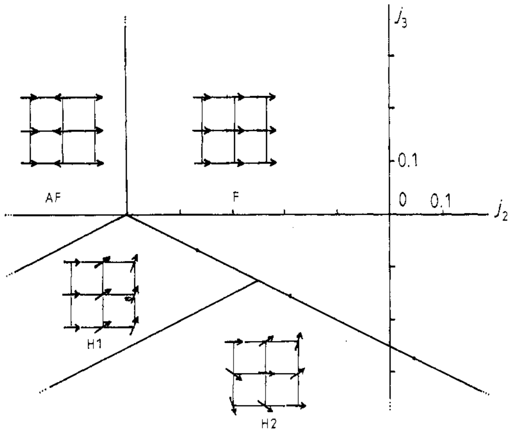

Figure 1. Phase diagram at zero temperature of the 3N classical tetragonal Heisenberg model: F, AF, H1, H2 refer to ferro-, antiferro-, and two the helical magnetic phases, respectively.

lattices. On the other hand a novel phase, where the helix wavevector changes continuously, spanning from the H1 to the H2 configuration, was found in the hexagonal lattice for in-plane interactions up to sixth-nearest neighbours [6]. Here we look for the existence of a similar phase, which we call a *swinging helix* (SH), in a tetragonal Heisenberg model.

The reduced energy of the tetragonal model for small helix wavevectors, reads

$$e(\boldsymbol{Q}) = E(\boldsymbol{Q})/4J_1NS^2$$
$$= e_0^{(0)} + e_1^{(0)}Q^2 + [e_2^{(0)} + e_2^{(1)}\cos(4\theta)]Q^4 + [e_3^{(0)} + e_3^{(1)}\cos(4\theta)]Q^6$$
$$+ [e_4^{(0)} + e_4^{(1)}\cos(4\theta) + e_4^{(2)}\cos(8\theta)]Q^8 \ldots \tag{2}$$

where $E(\boldsymbol{Q})$ is the energy of our model in a helical configuration, θ is the angle between $\boldsymbol{Q}$ and a NN direction. The conditions of minimum energy for a helix whose wavevector $\boldsymbol{Q}$ is directed neither along a NN (H1) nor along a NNN (H2) line, read

$$e_1^{(0)} + 2[e_2^{(0)} + e_2^{(1)}\cos(4\theta)]Q^2 + 3[e_3^{(0)} + e_3^{(1)}\cos(4\theta)]Q^4 + \ldots = 0 \tag{3a}$$

$$e_2^{(1)} + e_3^{(1)}Q^2 + [e_4^{(1)} + 4e_4^{(2)}\cos(4\theta)]Q^4 + \ldots = 0 \tag{3b}$$

$$e_2^{(0)} + e_2^{(1)}\cos(4\theta) + \ldots > 0 \tag{4a}$$

$$4(e_2^{(1)})^2 + 12e_2^{(1)}e_3^{(1)}Q^2 + [9(e_3^{(1)})^2 + 16e_2^{(1)}e_4^{(1)}$$
$$- 8e_2^{(0)}e_4^{(2)} + 56e_2^{(1)}e_4^{(2)}\cos(4\theta)]Q^4 + \ldots < 0. \tag{4b}$$

We look for solutions near the triple point F–H1–H2 corresponding to $e_1^{(0)} = e_2^{(1)} = 0$. At the lowest order in Q the solution of equations (3*a*) and (3*b*) is given by

$$Q^2 = e_1^{(0)}/2e_2^{(0)} = -e_2^{(1)}/e_3^{(1)} \tag{5}$$

where $e_2^{(0)}$ and $e_3^{(1)}$ have to be evaluated at the triple point.

Substitution of equation (5) into equations (4*a*) and (4*b*) gives

$$e_2^{(0)} > 0 \tag{6a}$$

$$(e_3^{(1)})^2 - 8e_2^{(0)}e_4^{(2)} < 0. \tag{6b}$$

At this point we have proved the possibility of having a non-conventional helix whose wavevector changes continuously its direction and magnitude between the H1 and H2 helical phases for a generic helimagnet with tetragonal symmetry. We stress that a similar configuration is a novelty in the scenario of the helimagnetism; this argument has been extensively studied in the last thirty years both experimentally and theoretically [7].

We shall now try to characterise this unorthodox SH phase in a tetragonal Heisenberg model with in-plane NN ferromagnetic interaction and competing exchange couplings up to fifth-nearest neighbours. We limit ourselves to this interaction scheme because it is sufficient to support the phenomenon in which we are interested.

We now give the relevant coefficients entering the reduced energy (2) where the interplane coupling J' is not accounted for, since its effect is simply to yield a ferromagnetic or antiferromagnetic interplane ordering depending on J' is positive or negative, respectively.

$$e_0^{(0)} = -1 - j_2 - j_3 - j_4 - j_5 \tag{7a}$$

$$e_1^{(0)} = (1/4)(1 + 2j_2 + 4j_3 + 5j_4 + 8j_5) \tag{7b}$$

$$e_2^{(0)} = -(3/4!8)(1 + 4j_2 + 16j_3 + 25j_4 + 64j_5) \tag{7c}$$

$$e_2^{(1)} = -(1/4!8)(1 - 4j_2 + 16j_3 - 7j_4 - 64j_5) \tag{7d}$$

$$e_3^{(1)} = (3/6!16)(1 - 8j_2 + 64j_3 - 35j_4 - 512j_5) \tag{7e}$$

$$e_4^{(2)} = -(1/8!128)(1 + 16j_2 + 256j_3 - 527j_4 + 4096j_5) \tag{7f}$$

where $j_\alpha = z_\alpha J_\alpha / z_1 J_1$, z being the coordination number. The F–H1–H2 triple point is given by

$$j_2 = -(1/4)(1 + 9j_4 + 32j_5) \tag{8a}$$

$$j_3 = -(1/8)(1 + j_4 - 16j_5). \tag{8b}$$

Equations (6*a*) and (6*b*) then become

$$1 - 7j_4 - 32j_5 > 0 \tag{9a}$$

$$j_4^2 + 2j_5(1 + j_4) < 0. \tag{9b}$$

For small j_4 and j_5 equation (9*a*) is always satisfied, while equation (9*b*) requires $j_5 < 0$. In order to find the region where the SH phase first occurs we come back to equations (3*a*) and (3*b*). By the definitions

$$\varepsilon = 4e_1^{(0)} \tag{10a}$$

$$\delta = 1 + 8j_3 + j_4 - 16j_5 \tag{10b}$$

equations (3*a*) and (3*b*) become

$$(1/4)\varepsilon + (1/4!4)Q^2[6(1 - 7j_4 - 32j_5) - 3(2\varepsilon + \delta) - (3\delta - 2\varepsilon)\cos(4\theta)] - (45/6!16)Q^4[3(1 - 11j_4 - 64j_5) + (1 + 5j_4 + 64j_5)\cos(4\theta)] = 0 \tag{11a}$$

$$-(1/4!8)(3\delta - 2\varepsilon) - (15/6!16)Q^2[1 + 5j_4 + 64j_5 + (1/5)(4\varepsilon - 10\delta)] + (7/8!32)Q^4[9(3 + 19j_4 + 384j_5) + 5(1 + 17j_4 - 128j_5)\cos(4\theta)] = 0. \tag{11b}$$

The solution of equations (11*a*) and (11*b*) is given by

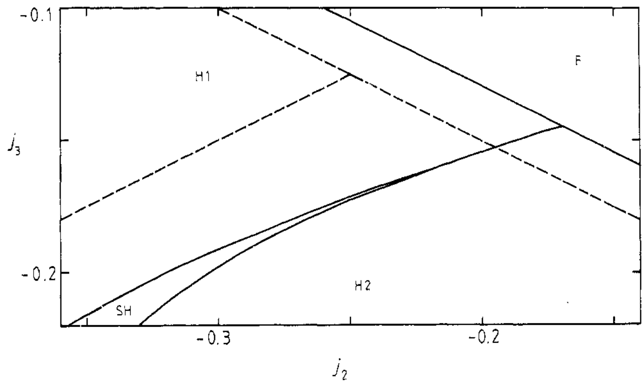

Figure 2. Wedge-shaped region of existence of the SH phase for $j_4 = 0$ and $j_5 = -0.01$. Broken lines refer to the phase diagram of the 3N model.

$$Q^2 = \alpha\delta + [\beta_0 + \beta_1 \cos(4\theta)]\delta^2 \tag{12}$$

$$\varepsilon = a\delta + [b_0 + b_1 \cos(4\theta)]\delta^2 \tag{13}$$

where

$$\alpha = -4/(1 - 3j_4) \qquad a = (1 - 7j_4 - 32j_5)/(1 - 3j_4) \tag{14a}$$

$$\beta_0 = -\frac{3 - 5j_4}{(1 - 3j_4)^3} \qquad b_0 = -\frac{12j_4(1 - 2j_4) + 8j_5(15 - 33j_4)}{3(1 - 3j_4)^3} \tag{14b}$$

$$\beta_1 = (1 + 9j_4)/3(1 - 3j_4)^3 \qquad b_1 = [4j_4^2 + 8j_5(1 + j_4)]/(1 - 3j_4)^3. \tag{14c}$$

As one can see in figure 2, equations (12) and (13) give the value of the $\boldsymbol{Q}$ wavevector of the novel SH phase as well as its wedge-shaped region of existence shown for $j_4 = 0, j_5 = -0.01$.

In summary we have shown that the degeneration line is destroyed by further exchange interactions, but that a phase in some sense reminiscent of the degenerate helix can arise in a wider parameter space. This novel phase consists of a narrow but finite wedge-shaped region where the helix wavevector assumes *all* possible directions.

We expect that the zero point motion (which is a dangerous mechanism as regards the survival of the DH phase [3, 8] in the SH phase should affect only the value of the energy of any SH configuration, so that this novel phase should not be removed by the zero point motion and it could be observed in real compounds.

An interesting point worthy of further investigation is the posssibility of exploring all SH configurations by application of an in-plane external magnetic field. This possibility has been proved to occur in the RAF model [9] where a particular helix out of the DH manifold is selected by an in-plane magnetic field. However, this conjecture requires further theoretical effort.

Acknowledgments

This work was supported in part by the Ministry of Education (MPI) and by the Gruppo Nazíonale Struttura della Materia (GNSM).

References

[1] Trullinger S E, Zakharov V E and Pokrovsky V L 1986 *Solitons* (Amsterdam: North-Holland)
[2] Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
[3] Rastelli E, Reatto L and Tassi A 1983 *J. Phys. C: Solid State Phys.* **16** L331
[4] Rastelli E and Tassi A 1986 *J. Phys. C: Solid State Phys.* **19** L423
[5] Rastelli E, Reatto L and Tassi A 1984 *Springer Series in Solid State Science* vol 54 (Berlin: Springer) p 195
[6] Harris A B, Rastelli E and Tassi A unpublished
[7] Coqblin B 1977 *The Electronic Structure of Rare Earth Metals and Alloys: The Magnetic Heavy Rare Earths* (London: Academic)
Adam A, Billerey D, Terrier C, Mainard R, Regnault L P, Rossat-Mignod J and Meriel P 1980 *Solid State Commun.* **35** 1
Day P and Ziebeck K R A 1980 *J. Phys. C: Solid State Phys.* **13** L523
Kuindersma S K, Sanchez J P and Haas C 1981 *Physica* B **11** 231
[8] Rastelli E and Tassi A 1987 *J. Phys. C: Solid State Phys.* **20** L303
[9] Rastelli E and Tassi A 1988 *J. Appl. Phys.* **63** 3823