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## A MAGNETIC ANALOGUE OF STEREOISOMERISM : APPLICATION TO HELIMAGNETISM IN TWO DIMENSIONS

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**Résumé.** — Les systèmes magnétiques invariants par un groupe de symétrie continu (tels que les modèles de Heisenberg ou XY) peuvent avoir un état fondamental à dégénérescence discrète, c'est-à-dire que les états de plus basse énergie forment dans l'espace de configuration des poches séparées par des barrières de potentiel. Ce phénomène est étudié en détail dans le cas d'un hamiltonien de spins isotrope sur un réseau de Bravais. Outre les verres de spin, dont nous ne parlons pas ici, une application de cette idée est le magnétisme à 2 dimensions : les systèmes magnétiques de Heisenberg dont l'état fondamental présente une dégénérescence discrète ont un certain type d'ordre à grande distance en dessous d'une certaine température de transition, alors que les ferromagnétiques bidimensionnels considérés habituellement sont désordonnés à toute température.

**Abstract.** — Magnetic systems invariant by a continuous symmetry group (e.g. the Heisenberg and XY models) may have a ground state which exhibits a discrete degeneracy, i.e. the lowest energy states form pockets separated by energy barriers in the phase space. This phenomenon is investigated in detail for the case of an isotropic, bilinear spin Hamiltonian on a Bravais lattice. Apart from spin glasses, which are not considered here, this idea can be applied to magnetism in two-dimensional lattices : two-dimensional, Heisenberg magnets with a discrete ground-state degeneracy are expected to have some kind of long range order below some transition temperature, whereas two-dimensional, conventional ferromagnets are disordered at all finite temperatures.

**1. Introduction.** — Broken symmetry is a current phenomenon in Nature : a system described by a Hamiltonian invariant under some symmetry group  $\mathcal{G}$  may have a ground state which is not invariant, but which is degenerate because any operation of  $\mathcal{G}$  transforms it into another state of lowest energy. In this paper, it is assumed that  $\mathcal{G}$  is a continuous group : in this case, the ground state can be continuously modified, at least in classical systems, and it can be said that it has a continuous degeneracy. But it may or may not happen that all states of lowest energy cannot be reached by continuous transformations of the ground state ; if they cannot, i.e. if states of lowest energy form pockets separated in the phase space by potential barriers, it will be said that the ground state has a discrete degeneracy, in addition to its continuous degeneracy. Well-known examples in chemistry are the stereoisomers of optically active molecules. However, this phenomenon does not seem to have been much investigated in magnetism, though it may be of some importance for spin glasses [1]. It has also important consequences for two-dimensional magnets, as will be seen in section 4.

A simple magnetic example is provided by a cluster of 4 classical spins  $S_A, S_B, S_C, S_D$  described by a Heisenberg Hamiltonian :

$$\mathcal{H} = -2J(S_B \cdot S_C + S_C \cdot S_D + S_D \cdot S_B) - 2J' S_A \cdot (S_B + S_C + S_D)$$

with  $J < 0$ . If  $|J'/J|$  is sufficiently small, an elementary calculation shows that there are 2 *stereoisomeric* ground states (Fig. 1) which cannot coincide by rotation.

In the present work, the ground state degeneracy is investigated for a periodic array of  $N$  classical,  $n$ -dimensional spins  $S_i$  of modulus  $\sqrt{S_i^2} = 1$ , sub-

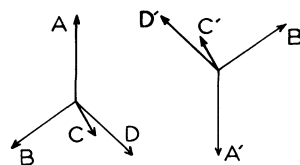


FIG. 1. — A finite magnetic system with a discrete ground state degeneracy. The C direction points into the paper and the C' direction points out.

mitted to an isotropic Hamiltonian, for instance a bilinear Hamiltonian :

$$\mathcal{H} = - \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j . \quad (1)$$

We shall assume  $n \geq 2$  throughout this paper. The cases  $n = 2$  (XY model) and  $n = 3$  (Heisenberg model) are of special interest for obvious physical reasons. The case  $n = 1$  (Ising model) will not be considered.

Sections 2 and 3 are devoted to the ground state degeneracy, and in section 4, this idea is applied to two-dimensional magnets at finite temperatures  $T \neq 0$ .

## 2. Bravais lattices with bilinear Hamiltonian. —

2.1 GENERAL FEATURES OF THE GROUND STATE. — If the spins are situated at the sites  $\mathbf{R}_i$  of a Bravais lattice, and if the Hamiltonian (1) acting on them has the corresponding translation invariance property, states of lowest energy are known [2] to be given, for  $n \geq 2$ , by :

$$\mathbf{S}_i = \mathbf{u} \cos \mathbf{Q} \cdot \mathbf{R}_i + \mathbf{v} \sin \mathbf{Q} \cdot \mathbf{R}_i \quad (2)$$

where  $\mathbf{u}$  and  $\mathbf{v}$  are 2 orthogonal, unit vectors and  $\mathbf{Q}$  is one of the absolute maxima of :

$$\mathcal{J}(k) = \sum_j J_{ij} \cos \mathbf{k}(\mathbf{R}_i - \mathbf{R}_j) . \quad (3)$$

Two values of  $\mathbf{Q}$  are *equivalent* if their difference is a reciprocal lattice vector. The set of non-equivalent values of  $\mathbf{Q}$  in the first Brillouin zone constitute the so-called *star* of  $\mathbf{Q}$ ; the star of  $\mathbf{Q}$  is a discrete set invariant under the symmetry operations of the point group [3].

2.2 FIRST CASE : THE STAR OF  $\mathbf{Q}$  CONSISTS OF ONLY ONE ELEMENT. — This case is the most common in Nature and is of no interest for the present work; it includes : i) ferromagnets (when  $\mathbf{Q} = 0$ ); ii) a class of antiferromagnets (when  $2\mathbf{Q}$  is a reciprocal lattice vector); classical antiferromagnets of this class can be transformed into ferromagnets by the transformation :

$$\boldsymbol{\sigma}_i = \mathbf{S}_i \cos \mathbf{Q} \cdot \mathbf{R}_i , \quad G_{ij} = J_{ij} \cos \mathbf{Q} \cdot (\mathbf{R}_i - \mathbf{R}_j) .$$

In this case, all states of lowest energy can be reached from one of them by a continuous rotation of the whole system of spins.

2.3 SECOND CASE : THE STAR OF  $\mathbf{Q}$  CONSISTS OF MORE THAN ONE ELEMENT. — This case is less common, but not exceptional in Nature [2, 4, 5]. For given values of  $\mathbf{u}$  and  $\mathbf{v}$ ,  $\mathbf{Q}$  can assume a finite number of discrete values, but the ground state has not necessarily a discrete degeneracy, because of two possible mechanisms :

i) The reversal of  $\mathbf{Q}$  in (2) is equivalent to the reversal of  $\mathbf{v}$ , and the latter can be done continuously, except for  $n = 2$ ; therefore, the ground state has no discrete degeneracy for  $n \geq 3$  if the star of  $\mathbf{Q}$  is reduced to  $\mathbf{Q}$  and  $-\mathbf{Q}$ .

ii) Equation (2) always describes lowest energy states, but not necessarily all of them; examples will be given at the end of this section.

It is shown in the appendix that all lowest energy states are described by (2), if  $n = 2$  or 3, except if  $\mathbf{Q}$  has certain special positions in the reciprocal space.

When all lowest energy states are given by (2), the ground state has a discrete degeneracy : i) for  $n = 3$  if the star of  $\mathbf{Q}$  is not reduced to  $\mathbf{Q}$  and  $-\mathbf{Q}$ ; ii) for  $n = 2$  if the star has more than one element.

An exhaustive list of the cases, where all lowest energy states are not described by eq. (2), will not be given here, and we shall be contented with a few examples.

a) Spin dimensionality  $n \geq 4$ . The simplest way to obtain a lowest energy state, which is not given by (2), is the *addition* of 2 states (2) with different structure vectors  $\mathbf{Q}$ ,  $\mathbf{Q}'$ , namely :

$$\mathbf{S}_i = (\mathbf{u} \cos \mathbf{Q} \cdot \mathbf{R}_i + \mathbf{v} \sin \mathbf{Q} \cdot \mathbf{R}_i) \cos \theta + (\mathbf{w} \cos \mathbf{Q}' \cdot \mathbf{R}_i + \mathbf{m} \sin \mathbf{Q}' \cdot \mathbf{R}_i) \sin \theta \quad (4)$$

where  $\theta$  is an arbitrary phase,  $\mathbf{u}$ ,  $\mathbf{v}$ ,  $\mathbf{w}$ ,  $\mathbf{m}$  are 4 unit vectors, which must be orthogonal to satisfy the condition  $|\mathbf{S}_i|^2 = 1$ .  $\mathbf{Q}$  can be continuously changed into  $\mathbf{Q}'$  by varying  $\theta$  from 0 to  $\pi/2$ .

b) If  $2\mathbf{Q} = \boldsymbol{\tau}$  is a reciprocal lattice vector,  $\sin \mathbf{Q} \cdot \mathbf{R}_i = \sin \mathbf{Q}' \cdot \mathbf{R}_i = 0$ , so that  $\mathbf{v}$  and  $\mathbf{m}$  disappear from equation (4), and only 2 orthogonal, unit vectors  $\mathbf{u}$  and  $\mathbf{w}$  are required; equation (4) now reads :

$$\mathbf{S}_i = \mathbf{u} \cos \mathbf{Q} \cdot \mathbf{R}_i \cos \theta + \mathbf{w} \cos \mathbf{Q}' \cdot \mathbf{R}_i \sin \theta . \quad (5)$$

These states exist for all values of  $n \geq 2$ ; again the transition from  $\mathbf{Q}$  to  $\mathbf{Q}'$  can be done by a continuous transformation.

c) If  $4\mathbf{Q} = \boldsymbol{\tau}$  is a reciprocal lattice vector, and is  $2\mathbf{Q}$  is not, this is again possible for  $n \geq 2$ , though it is not obvious from (2). This can be explained as follows : let  $F$  be the set of spins parallel to  $\mathbf{u}$  in the state (2), and let  $G$  be the set of spins parallel to  $\mathbf{v}$  : the spins  $F$  see no field produced by the spins  $G$  (and *vice versa*); this is obvious, because otherwise the spins would align parallel to the same direction. Therefore, it is possible to tilt the spins  $G$  without energy change :

$$\mathbf{S}_i = \mathbf{u}(\cos \mathbf{Q} \cdot \mathbf{R}_i + \sin \mathbf{Q} \cdot \mathbf{R}_i \cos \psi) + \mathbf{v} \sin \mathbf{Q} \cdot \mathbf{R}_i \sin \psi . \quad (6a)$$

In particular, the spins can be aligned ( $\psi = 0$ ), and then it is possible to *add* two states with different values of  $\mathbf{Q}$ , obtaining a state described by :

$$\mathbf{S}_i = \mathbf{u}(\cos \mathbf{Q} \cdot \mathbf{R}_i + \sin \mathbf{Q} \cdot \mathbf{R}_i) \cos \theta + \mathbf{v}(\cos \mathbf{Q}' \cdot \mathbf{R}_i + \sin \mathbf{Q}' \cdot \mathbf{R}_i) \sin \theta. \quad (6b)$$

Again  $\mathbf{Q}$  can be changed into  $\mathbf{Q}'$  by the continuous transformation of  $\theta$  from 0 to  $\pi/2$ .

*Remarks :*

i) Cases (b) and (c) involve colinear structures (in addition to canted structures) which can be considered as *starred* antiferromagnets. Colinear structures can be obtained only for  $\mathbf{Q} = 0$  or  $2\mathbf{Q} = \boldsymbol{\tau}$  or  $4\mathbf{Q} = \boldsymbol{\tau}$ , where  $\boldsymbol{\tau}$  is a reciprocal lattice vector ; Cases  $3\mathbf{Q} = \boldsymbol{\tau}$  or  $6\mathbf{Q} = \boldsymbol{\tau}$ , for instance, have no special properties.

ii) Cases (a), (b), (c) are not the only examples of structures not described by (2) ; another example of minor experimental interest is provided by the case when  $2\mathbf{Q}$  lies on a Brillouin zone boundary, for certain symmetries.

iii) The values  $\mathbf{Q} = 0, \tau/2$  and  $\tau/4$  are favoured by symmetry [18], as well as  $\mathbf{Q} = \tau/3$  or  $\tau/6$ , for certain lattices. Other commensurable values are not favoured for purely isotropic interactions and can only occur accidentally.

iv) The absence of discrete ground state degeneracy in the above examples (a), (b), (c) is a pathological feature of the bilinear Hamiltonian (1) ; biquadratic terms, for instance, restore the discrete degeneracy, as will be seen in section 3.

v) When all lowest energy states are given by (2), the discrete degeneracy of the ground state is easily seen to be  $2m$  for  $n = 2$ , and  $m$  for  $n = 3$ , if  $2m$  is the number of elements of the star of  $\mathbf{Q}$ .

**2.4 ORDER PARAMETER.** — When the lowest energy states split into several continuous sets separated by potential barriers, the various sets can be characterized by the corresponding values of  $\mathbf{Q}$  ; however, it is preferable, in order to extend the theory to finite temperatures  $T \neq 0$ , to define a local, observable order parameter, as a function of the field  $\mathbf{S}_i$ .

For  $n = 2$ , such an order parameter is the following quantity, which is a vector in the lattice space, with  $D$  components which are pseudo-scalars in the spin-space :

$$Q_i^\alpha = \mathbf{S}_i \times \partial_\alpha \mathbf{S}_i \quad (7)$$

where  $\alpha = x, y, z$  ;  $\partial_\alpha \mathbf{S}_i$  is defined for the cubic lattice by :

$$\mathbf{S}_i(\mathbf{R}_i + \mathbf{a}_\alpha) - \mathbf{S}_i(\mathbf{R}_i) = a \partial_\alpha \mathbf{S}_i$$

where  $a_x, a_y$ , and  $a_z$  are the interatomic vectors along  $x, y, z$ .

At  $T = 0$ , the quantity  $\mathbf{Q}_i$  defined by (7) reduces to :

$$\frac{1}{a} (\sin Q_x a, \sin Q_y a, \sin Q_z a)$$

and its knowledge is equivalent to the knowledge of  $\mathbf{Q}$ , except if  $Q_x$  or  $Q_y$  or  $Q_z$  is equal to  $\pi/2 a$ .

For  $n \geq 3$ , no pseudo-scalar similar to (7) can be derived from the two-dimensional field (2), but a possible order parameter is the following  $D \times D$  tensor, whose components are scalars in the spin-space :

$$q_i^{\alpha\gamma} = (\partial_\alpha \mathbf{S}_i) \cdot (\partial_\gamma \mathbf{S}_i). \quad (8)$$

At  $T = 0$ , the knowledge of  $q_i^{\alpha\gamma}$  is equivalent to the knowledge of  $\mathbf{Q}$ , except for certain special positions of  $\mathbf{Q}$ .

The difference between Heisenberg and XY models is related to the difference which was noticed in section 2.3.

**3. Bravais lattice with biquadratic interactions.** — Biquadratic interactions are the simplest sophistication of the model (1), which does not violate the isotropic character. The Hamiltonian becomes :

$$\mathcal{H} = - \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{i,j} g_{ij} (\mathbf{S}_i \cdot \mathbf{S}_j)^2. \quad (9)$$

There is no general recipe for the ground state. It can happen, however, that the classical ground state is still given by (2). In particular, positive  $g_{ij}$ 's stabilise colinear states encountered in section 2.3 :  $\theta = 0$  or  $\pi/2$  in eq. (5) and (6b),  $\psi = 0$  in (6a). More generally, biquadratic interactions can restore the discrete degeneracy of the ground state.

Results from sections 2 and 3 are summarised in table I.

TABLE I

*Existence (Yes) or non-existence (No) of a discrete ground-state degeneracy for Bravais lattices having a state of lowest energy described by equation (2). In cases denoted by a star, biquadratic terms are necessary for a discrete ground state degeneracy. The list is not exhaustive.*

	Star of $\mathbf{Q}$ reduced to $\mathbf{Q}$ and $-\mathbf{Q}$	Star of $\mathbf{Q}$ not reduced to $\mathbf{Q}$ and $-\mathbf{Q}$
$\mathbf{Q}$ is not in a special position	$n = 2$ Yes $n = 3$ No $n \geq 4$ No	Yes Yes Yes (*)
$4\mathbf{Q}$ is a reciprocal lattice vector but $2\mathbf{Q}$ is not	$n = 2$ Yes (*) $n \geq 3$ Yes (*) for colinear structures No for states described by [2]	Yes (*)
$2\mathbf{Q}$ is a reciprocal lattice vector	(Nonsense)	Yes (*)

An interesting case, for  $n = 3$ , is when the ground state is not described by eq. (2), but instead contains Fourier components  $\mathbf{Q}$ ,  $\mathbf{Q}'$ ,  $\mathbf{Q}''$  which do not belong all to the same star; an example is provided by Erbium, where  $\mathbf{Q}' = -\mathbf{Q}$  and  $\mathbf{Q}'' = 0$ :

$$\mathbf{S}_R = (\mathbf{u} \cos \mathbf{Q} \cdot \mathbf{R} + \mathbf{v} \sin \mathbf{Q} \cdot \mathbf{R}) \sin \theta + \mathbf{w} \cos \theta \quad (10)$$

The essential difference with the cases considered in section 2 is that there is a discrete, double degeneracy for  $n = 3$  even if the star of  $\mathbf{Q}$  is reduced to  $\mathbf{Q}$  and  $-\mathbf{Q}$ , since it is impossible to transform  $\mathbf{Q}$  into  $-\mathbf{Q}$  in (10) by a continuous transformation without crossing an energy barrier. A possible order parameter is the following set of 2 pseudo-scalar components:

$$\tau_i^\alpha = \mathbf{M}_i \cdot (\mathbf{S}_i \times \partial_\alpha \mathbf{S}_i) \quad (11)$$

where

$$\mathbf{M}_i = \sum_j g_{ij} \mathbf{S}_j$$

where  $g_{ij} = 1$  for nearest neighbours,  $g_{ij} = 0$  otherwise.

The structure (10) can be produced by anisotropic forces, but also by biquadratic, isotropic exchange. Similar structures with Fourier components  $\mathbf{Q}$ ,  $-\mathbf{Q}$  and 0 can also result from bilinear, isotropic exchange forces in non-Bravais lattices.

So far, only the ground state properties have been considered in this paper. In the next sections, the consequences of a discrete ground state degeneracy on the properties of two-dimensional magnets at finite temperature are investigated.

**4. Application to magnetism in two-dimensional lattices.** — 4.1 THE MERMIN-WAGNER THEOREM AND THE SPIN-PAIR CORRELATION FUNCTION. — The theorem established by Mermin and Wagner [6] for ferromagnets and antiferromagnets can easily be extended to all magnets described by the Hamiltonian (1) for  $n = 3$  and short range interactions, on a two-dimensional lattice: the Mermin-Wagner theorem states that the staggered magnetisation:

$$\langle \mathbf{M}_Q \rangle = N^{-1} \sum_i \langle \mathbf{S}_i \rangle \exp i\mathbf{Q} \cdot \mathbf{R}_i$$

has a vanishing limit at all finite temperatures when the applied staggered field goes to zero.

In the ferromagnetic case, it is commonly admitted that the spin pair correlation function  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  has a limit when the distance  $r_{ij}$  goes to infinity. This limit is obviously  $\langle \mathbf{S}_i \rangle^2$ , and the Mermin-Wagner theorem implies that it is zero for two-dimensional lattices if  $T \neq 0$ :

$$\lim_{r_{ij} \rightarrow \infty} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = 0. \quad (12)$$

We suggest that all two-dimensional, isotropic magnets with  $n \geq 2$ , have the property (12), whatever be their structure (ferromagnetic, antiferromagnetic, helimagnetic...). For  $n = 2$ , the property (12) results from any approximation, for instance the harmonic approximation, proposed by Wegner [7] for ferromagnets, and which can easily be extended to helimagnets (i.e. structures given by eq. (2) when  $2\mathbf{Q} \neq \boldsymbol{\tau}$ ); the extension of the statement (12) to higher values of  $n$  is justified by the fact that the increase of  $n$  is expected to increase fluctuations, and therefore to decrease correlations. Eq. (12) can be proved for  $n = \infty$  (spherical model).

4.2 PHASE TRANSITIONS IN TWO-DIMENSIONAL, HEISENBERG OR XY MAGNETS. — We shall now argue that two-dimensional magnetic systems which have a discrete ground state degeneracy do exhibit some kind of long range order (L.R.O.) at low temperature, and therefore have a transition at some temperature  $T_c$ . More precisely, the XY helimagnet considered in section 2.3 c) satisfies for  $T < T_c$  the property:

$$\lim_{r_{ij} \rightarrow \infty} \langle \mathbf{Q}_i^\alpha \mathbf{Q}_j^\alpha \rangle = f_\alpha(T) \neq 0 \quad (13)$$

where  $\mathbf{Q}_i^\alpha$  is defined by (7). The Heisenberg helimagnet described in section 2.3 d) satisfies for  $n = 3$  the property:

$$\lim_{r_{ij} \rightarrow \infty} \langle q_i^{\alpha\gamma} q_j^{\alpha\gamma} \rangle = f_{\alpha\gamma}(T) \neq 0 \quad (14)$$

where  $q_i^{\alpha\gamma}$  is defined by (8). The system described by (10) at  $T = 0$  has below  $T_c$  the property:

$$\lim_{r_{ij} \rightarrow \infty} \langle \tau_i^\alpha \tau_j^\alpha \rangle = f_\alpha(T) \neq 0 \quad (15)$$

where  $\tau_i^\alpha$  is defined by (11). Properties (13) to (15) do not contradict equation (12) nor the Mermin-Wagner theorem.

4.3 THE ARGUMENT. — For properties (13) to (15) at low temperatures, is as follows. For definiteness, we shall argue on the XY helimagnet (eq. (13)) but the argument is general.

First, if  $K_B T$  is much lower than the typical exchange interaction  $|J|$ ,  $\mathbf{Q}_i$  is nearly equal to one of the maxima of  $\mathcal{J}(\mathbf{k})$  at nearly all sites (<sup>1</sup>). This can be seen from a standard spin-wave calculation in a *finite* volume  $\mathcal{V}$  containing  $L^2$  unit cells. This calculation will not be explicitly given here, but it is quite similar to that of Berezinskii and Blank [8] for ferromagnets. It starts with the assumption that  $\mathbf{S}_i$  is given by the expression (2), plus small deviations  $\delta\mathbf{S}_i$ ; neglecting third and higher order terms in  $\delta\mathbf{S}_i$  in the Hamiltonian, one

(<sup>1</sup>) This argument is for a continuous model, when  $\mathbf{Q}_i$  is defined by (7) again, but  $\partial_\alpha \mathbf{S}_i$  is an ordinary gradient; in this case,  $\mathbf{Q}_i$  reduces to  $\mathbf{Q}$  at  $T = 0$ . The extension to a lattice only implies a change of vocabulary.

calculates  $\langle \delta S_i^2 \rangle$ , which is indeed found to be small if  $L \ll \exp |J|/K_B T$ , the self-consistency condition. The fluctuation  $\langle (\mathbf{Q}_i - \mathbf{Q})^2 \rangle$  is calculated in the same way and is also found to be small, so that  $\mathbf{Q}_i$  is almost equal to one of the maxima  $\mathbf{Q}$  of  $\mathfrak{J}(\mathbf{k})$  at almost all sites  $i$ .

This statement is also expected to be true at low temperature for an infinite magnet, since an infinite magnet can be considered as an assembly of interacting cells of size  $L^2$ , and the interactions can just increase the tendency that  $\mathbf{Q}_i$  lies close to one of the maxima of  $\mathfrak{J}(\mathbf{k})$ .

There are, however, a few sites at which  $\mathbf{Q}_i$  is *not* close to one of the maxima of  $\mathfrak{J}(\mathbf{k})$ ; the problem is : can these few sites destroy L.R.O., i.e., can they make equation (13) wrong ? Clearly, they can only destroy L.R.O. if they are concentrated in frontiers separating regions having different values of  $\mathbf{Q}$ . For a discrete order parameter, frontiers must be narrow at low temperatures since their entropy is irrelevant and their energy is proportional to their thickness. The energy of a narrow frontier per unit length is of order  $|J|$ , and its entropy is of order  $K_B$ . Therefore the ordered state (when  $\mathbf{Q}_i$  is close to the same element  $\mathbf{Q}$  of the star at almost each site) is stable with respect to the formation of one frontier, provided  $K_B T \lesssim |J|$ . A long range ordering of the type described in section 4.2 is therefore expected below a transition temperature of order :

$$K_B T_c \approx |J|. \quad (16)$$

4.4 DISCUSSION. — We have given a rather rough argument, for the sake of brevity and simplicity, but it can easily be improved; also note that it can easily be extended to quantum systems. It can also be extended to 3-dimensional spins with an XY anisotropy, and in this case, the semi-polar representation [9] can be used, with the advantage that the spin-wave calculation can be performed in an infinite sample at once. In the Heisenberg case, however, the method of section 4.3 is the only one which can be applied.

Also for the sake of simplicity, we have given the order of magnitude (16) as a general result; this is not strictly true; more generally,  $K_B T_c$  is expected to be of order  $\Delta$ , where  $\Delta$  is the energy barrier between the various maxima of  $\mathfrak{J}(\mathbf{k})$ . It can happen that  $\Delta$  is appreciably lower than  $|J|$ , for instance near a Lifshitz point [10, 11, 12, 13] and this probably explains why the Néel temperature of the (expectedly quasi-two-dimensional) helimagnet  $\text{BaCo}_2(\text{AsO}_4)_2$  is much lower than the average exchange interaction  $|J|$  (see ref. [14] and [15]).

A possible approach to helimagnets has been described by Mukamel *et al.* [4] and by Garel [5], who show that within the Landau-Wilson formulation a helimagnet is equivalent to an *anisotropic* ferromagnet with  $(2nm)$ -dimensional spins, if  $2m$  is the

number of elements of the star of  $Q$ ; in this approach, the possibility of L.R.O. at low temperature would probably result from the anisotropy.

A final remark is that a transition is expected at a temperature of order  $|J|/K_B$  for two-dimensional ferromagnets of the XY type [16], but this transition involves no long range ordering, in contrast with properties (13) to (15). The ordering described in this section is even more spectacular for Heisenberg systems, since conventional, Heisenberg ferromagnets are presently believed to have no transition [17].

## APPENDIX

**Discrete degeneracy of the ground state of the Heisenberg model on a Bravais lattice, when the structure vector  $\mathbf{Q}$  is not in a special position.** — It is easily shown [2] that the classical ground state of (1) on a Bravais lattice is the solution of the system :

$$\mathbf{S}_i = \sum_{\mathbf{Q}} \mathbf{x}_{\mathbf{Q}} \exp i\mathbf{Q} \cdot \mathbf{R}_i \quad (\text{A.1})$$

$$\mathbf{S}_i = \mathbf{S}_i^* \quad (\text{A.2})$$

$$|\mathbf{S}_i|^2 = 1. \quad (\text{A.3})$$

The summation in (A.1) is over the elements of the star of the maxima of (3). Eq. (A.2) yields :

$$\mathbf{x}_{\mathbf{Q}} = \mathbf{x}_{-\mathbf{Q}}^*. \quad (\text{A.4})$$

Eq. (A.4) yields, after insertion of (A.1) :

$$\sum_{\mathbf{Q}, \mathbf{Q}'} (\mathbf{x}_{\mathbf{Q}} \cdot \mathbf{x}_{\mathbf{Q}'}^*) \exp i(\mathbf{Q} - \mathbf{Q}') \cdot \mathbf{R}_i = 1 \quad (\text{A.5})$$

or :

$$\sum_{\tau} \sum_{\mathbf{Q}, \mathbf{Q}'} (\mathbf{x}_{\mathbf{Q}} \cdot \mathbf{x}_{\mathbf{Q}'}^*) \delta_{\mathbf{Q}, \mathbf{Q} + \mathbf{k} + \tau} = \delta_{0, \mathbf{k}} \quad (\text{A.5})$$

where the sum is over the elements  $\mathbf{Q}, \mathbf{Q}'$  of the star and over the reciprocal lattice vectors  $\tau$ .

When  $\mathbf{Q}' = -\mathbf{Q}$ , there is generally only one term in the sum at the L.H.S. of (A.5). The exception is when there are 3 elements  $\mathbf{Q}, \mathbf{Q}', \mathbf{Q}''$  of the star, which satisfy :

$$\mathbf{Q}' + \mathbf{Q}'' = 2\mathbf{Q} + \tau. \quad (\text{A.6})$$

This equation can only be satisfied if  $\mathbf{Q}$  has a particular position; for instance, if  $4\mathbf{Q} = \tau$  (A.6) is satisfied for  $\mathbf{Q}' = \mathbf{Q}'' = -\mathbf{Q}$ ; it will be assumed, from now on, that (A.6) is not satisfied by any 3 vectors of the star. In this case, insertion of  $\mathbf{Q}' = -\mathbf{Q}$  into (A.5) yields :

$$\mathbf{x}_{\mathbf{Q}} \cdot \mathbf{x}_{-\mathbf{Q}}^* = x_{\mathbf{Q}}^2 = 0$$

or :

$$\mathbf{x}_{\mathbf{Q}} = y_{\mathbf{Q}}(\mathbf{u}_{\mathbf{Q}} + i\nu_{\mathbf{Q}}) \quad (\text{A.7})$$

where  $y_Q$  is a real number,  $\mathbf{u}_Q$  and  $\mathbf{v}_Q$  are orthogonal unit vectors. According to (A.4), one can choose :

$$\mathbf{u}_Q = \mathbf{u}_{-Q}, \quad y_Q = y_{-Q}, \quad \mathbf{v}_Q = -\mathbf{v}_{-Q}. \quad (\text{A.8})$$

When  $\mathbf{Q}' \neq -\mathbf{Q}$ , the sum at the L.H.S. of (A.5) generally consists of several terms, and the discussion should be continued separately for each type of symmetry ; the forthcoming discussion assumes that  $\mathbf{Q}$  is in general position ; in this case, the summation over  $\tau$  in (A.5) can be limited to  $\tau = 0$ .

a) *Monoclinic lattice.* — The star consists of 4 vectors  $\pm \mathbf{Q}_1, \pm \mathbf{Q}_0$ , which form a rectangle. One of the two quantities  $y_0, y_1$  can be assumed to be different from zero, for instance  $y_0 \neq 0$ . If, in addition,  $y_1 \neq 0, \mathbf{u}_0, \mathbf{u}_1, \mathbf{v}_0, \mathbf{v}_1$  must satisfy the following set of equations, which is easily deduced from (A.5) :

$$\mathbf{u}_0 \cdot \mathbf{u}_1 = \mathbf{v}_0 \cdot \mathbf{v}_1 = \mathbf{u}_0 \cdot \mathbf{v}_1 = \mathbf{u}_1 \cdot \mathbf{v}_0 = 0. \quad (\text{A.9})$$

In addition,  $\mathbf{u}_0 \cdot \mathbf{v}_0 = \mathbf{u}_1 \cdot \mathbf{v}_1 = 0$ . This system has solutions for  $n \geq 4$ , and they correspond to the structure (4). For  $n = 2$  or 3, (A.9) has no solution, therefore  $y_1 = 0$  : this corresponds to equation (2).

b) *Orthorhombic lattices.* — The star consists of 8 elements :  $\pm \mathbf{Q}_0, \pm \mathbf{Q}_1, \pm \mathbf{Q}_2, \pm \mathbf{Q}_3$ ; let  $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3$  be deduced from  $\mathbf{Q}_0$  by symmetries through 3 orthogonal planes; assuming  $y_0, y_1, y_2 \neq 0$ , one deduces from (A.5) the following homogeneous equations :

$$\begin{aligned} \mathbf{u}_0 \cdot \mathbf{u}_1 - \mathbf{v}_0 \cdot \mathbf{v}_1 &= \mathbf{u}_0 \cdot \mathbf{u}_2 - \mathbf{v}_0 \cdot \mathbf{v}_2 = \\ &= \mathbf{u}_1 \cdot \mathbf{u}_2 + \mathbf{v}_1 \cdot \mathbf{v}_2 = 0 \\ \mathbf{u}_0 \cdot \mathbf{v}_1 + \mathbf{u}_1 \cdot \mathbf{v}_0 &= \mathbf{u}_0 \cdot \mathbf{v}_2 + \mathbf{u}_2 \cdot \mathbf{v}_0 = \\ &= \mathbf{u}_1 \cdot \mathbf{v}_2 - \mathbf{u}_2 \cdot \mathbf{v}_1 = 0. \end{aligned}$$

In view of the orthogonality of  $\mathbf{u}$  and  $\mathbf{v}$ , it is easily seen that these relations cannot be satisfied by unit vectors ; therefore, one of the  $y_k$ 's is zero, for instance  $y_2 = 0$ ; but, in this case, the argument (b) can be applied to  $\mathbf{Q}_0, -\mathbf{Q}_0, \mathbf{Q}_1$  and  $-\mathbf{Q}_1$ , and yields  $y_0 = 0$  or  $y_1 = 0$ ; the same argument as above holds if  $\mathbf{Q}_2$  is replaced by  $\mathbf{Q}_3$ . The final result is that only one of the 4 numbers  $y_0, y_1, y_2, y_3$  can be different from zero, so that all lowest energy states have the form (2), when  $n = 2$  or 3.

c) *Tetragonal lattices.* — The star consists of 16 elements ; let  $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3$  be deduced from  $\mathbf{Q}_0$  by rotations of  $\pi/2, \pi$  and  $3\pi/2$  around the tetragonal axis,

and let  $\pm \mathbf{Q}'_0, \pm \mathbf{Q}'_1, \pm \mathbf{Q}'_2$  and  $\pm \mathbf{Q}'_3$  be the other elements. According to the same argument as in b),  $y_1$  and  $y_3$  should vanish if  $y_0 \neq 0$ ;  $y'_1$  and  $y'_3$  also vanish if one assumes  $y'_0 \neq 0$ , for instance, if

$$y_1 = y'_1 = y_3 = y'_3 = 0,$$

the argument b) can be applied to show that not more than one of the 3 quantities  $y_0, y'_0, y_2, y'_2$  can be different from zero if  $n \leq 3$ , so that all lowest energy states have the form (2).

d) *Hexagonal lattice.* — In the general case, the star of  $\mathbf{Q}$  consists of 24 vectors : let  $\mathbf{Q}_1, \dots, \mathbf{Q}_{11}$  be deduced from  $\mathbf{Q}_0$  by rotations around the hexagonal axis  $c$ , and by symmetries through planes parallel to  $c$ ; let  $\mathbf{Q}_{p+6}$  be symmetric of  $\mathbf{Q}_p$  with respect to the  $c$  axis ; assume  $y_0 \neq 0$  ; then the argument b) can be applied to the 8 vectors  $\pm \mathbf{Q}_0, \pm \mathbf{Q}_6, \pm \mathbf{Q}_p, \pm \mathbf{Q}_{p+6}$  to show that  $y_p = 0$  for all  $p \neq 0$  or 6 ; finally the argument a) can be applied to the 4 vectors  $\pm \mathbf{Q}_0$  and  $\pm \mathbf{Q}_6$  to show that  $y_6$  also vanishes. The reason why  $y_6$  should be considered at the end of the argument is that there are many vectors  $(\mathbf{Q}, \mathbf{Q}')$  satisfying  $\delta_{\mathbf{Q}, \mathbf{Q} + \mathbf{Q}_0 + \mathbf{Q}_6} \neq 0$ , so that the term containing  $y_0 y_6$  is associated to many other terms in (A.5). Again, all lowest energy states are described by (2) if  $n = 2$  or 3.

e) *Rhombohedral lattice.* — The star of  $\mathbf{Q}$  is reduced to 12 elements and can be deduced from the star corresponding to the hexagonal lattice, by the suppression of 12 vectors, or, alternatively, by the requirement that the corresponding  $y_p$ 's vanish ; therefore, the conclusion that only one of the  $y_p$ 's can be different from zero, remains correct.

f) *Cubic lattices.* — The proof is analogous but tedious.

g) *Exceptions.* — The argument applies whenever it is impossible to find 4 vectors  $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \mathbf{Q}_4$  of the star, which satisfy :

$$\mathbf{Q}_1 + \mathbf{Q}_2 + \mathbf{Q}_3 + \mathbf{Q}_4 = \tau \quad (\text{A.10})$$

where  $\tau$  is a reciprocal lattice vector. (A.10) is a generalization of (A.6), since (A.5) corresponds to  $\mathbf{Q}_3 = \mathbf{Q}_4$ .

The fact that  $\mathbf{Q}$  eventually lies on a symmetry plane or axis apparently does not change the general result, since this does not imply that (A.10) is satisfied.

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