DETERMINATION OF MAGNETIC STRUCTURES USING THE LANDAU THEORY OF SECOND ORDER PHASE TRANSITIONS

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Résumé. — Un aperçu de la théorie de Landau sur les transitions de phases du second ordre est présenté. Son application à la détermination de structures magnétiques possibles d'un cristal y trouve une attention spéciale. Les restrictions sur le changement de symétrie sont analysées par la théorie des groupes. Il est montré que pour des structures simples la symétrie peut être déterminée sans théorie des groupes. Les transitions entre deux états magnétiques sont aussi discutées.

Abstract. — A review of Landau's theory of second order phase transitions is given with special emphasis on its application to determine the possible magnetic structures that can arise when a paramagnetic crystal undergoes a magnetic phase transition. Using group theoretical methods the restrictions for the change of the magnetic symmetry are outlined. It is shown that for not too complicated magnetic structures the symmetry can be determined without group theoretical calculations. Second order phase transitions between two magnetic phases are also discussed.

I. Introduction. — The investigation of the magnetic symmetry of a crystal represents a special topic in the field of magnetic phenomena. Experimentally in fitting the data of a neutron diffraction pattern usually a variety of structures is taken as « trial structures », among which the fit has to choose the real one. In most of the works the choice of the « trial structures » is accidental and is not based on theoretical expectations. Theoretically an unequivocal determination of the magnetic symmetry is feasible only in the knowledge of all the exchange and anisotropic forces, which usually are not available.

There is, however, a possibility, at least for second order phase transitions, using only symmetry considerations, to determine the structures that can arise when a paramagnetic crystal with given symmetry undergoes a magnetic phase transition. Only these structures have to be considered as « trial structures » and this limits their number. This method is based on an extension of Landau's thermodynamic theory of second order phase transitions [1]. This theory, as it is known, gives not only the temperature behaviour of the thermodynamic quantities, but also predicts the symmetry of the new phase. Actually Landau's original paper [2] contains all the ideas how the change in the symmetry has to be determined. The first applications to non-magnetic (ordered alloys) and magnetic systems have been given by Lifshitz [3] and Dzyaloshinskii [4], respectively. The first great success of the theory in this respect was the explanation of the existence of weak ferromagnetism [4]. Since then there have been several attempts to perform a systematic investigation of the possible magnetic phase transitions. The most important contribution has been made by Kovalev [5], who has found a new criterion in selecting the irreducible representations capable of describing magnetic structures.

In Sec. II we will give a general formulation of the problem for paramagnetic-magnetic phase transitions. The question we address ourselves to is what kind of magnetic structures can occur in a crystal having a given non-magnetic space group. We will list without mathematical proof the criteria that restrict the possible symmetry changes and show how the minimization of the thermodynamic potential can yield the allowed magnetic structures. In this treatment we will rely on group theory. It will be shown in Sec. III, that for not too complicated structures the calculation can be done without the apparatus of group theory. In Sec. IV we will shortly discuss phase transitions between two magnetic phases, this calculation being a simple generalization of that for paramagnetic-magnetic transitions. Finally in Sec. V the main steps in the determination of the magnetic symmetry will be summarized.

II. Formulation of the problem for paramagnetic-magnetic phase transitions. — The main point in the Landau theory is that in second order phase transitions there always exists an order parameter, which in one of the phases is identically zero, while in the other one it has finite value. For magnetic phase transitions the order parameter is the staggered magnetization. The variation of the order parameter is continuous at the transition temperature T_c yielding, however, a discontinuous change in the symmetry of the system. The order parameter being small in the neighbourhood of T_c the thermodynamic potential Φ can be expanded in its powers. If $M(r)$ denotes the magnetic moment density, the above statement means that

$$\Phi(p, T, M(r)) = \Phi_0(p, T) + \Phi_1(p, T, M(r)) + \\ + \Phi_2(p, T, M(r)) + \cdots , \quad (1)$$

where $\Phi_i(p, T, M(r))$ is an ith order functional of $M(r)$. Our task is to specify these functions using only general group theoretical arguments.

Let G_0 be the crystallographic space group of the crystal in the paramagnetic phase and let R denote the operation of time reversal as well as the group containing the unit element E and R. The magnetic space group of the paramagnetic phase is the direct product of the groups G_0 and R ($G_0 \otimes R$). Supposing that all the irreducible representations $T^{(k,m)}$ and basis functions $\psi_i^{(k,m)}$ of this group are known, $M(r)$ can be expressed as a linear combination of these basis functions in the following form

$$M(r) = \sum_\alpha \sum_{k,m,i} \mathbf{e}_\alpha \, c_{i,\alpha}^{(k,m)} \, \psi_i^{(k,m)} , \quad (2)$$

where $\mathbf{k}$ denotes a vector of the star of the representation, m refers to the mth irreducible representation belonging to the given star, while i refers to the ith

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basis function of the representation and e_α is the unit axial vector in the direction α ($\alpha = x, y, z$).

Inserting eq. (2) into Φ_i of eq. (1) we get

$$\Phi_1(p, T, M(r)) = \sum_\alpha \sum_{k,m,i} c_{i,\alpha}^{(k,m)} \Phi_1(p, T, e_\alpha \psi_i^{(k,m)}(r))$$

$$\Phi_2(p, T, M(r)) = \sum_{\alpha,\alpha'} \sum_{k,m,i} \sum_{k',m',i'} c_{i,\alpha}^{(k,m)} c_{i'\alpha'}^{(k',m')} \times$$

$$\times \Phi_2(p, T, e_\alpha \psi_i^{(k,m)}(r), e_{\alpha'} \psi_{i'}^{(k',m')}(r)) . \quad (3)$$

The thermodynamic potential $\Phi(p, T, M(r))$ is expressed as a power series of the parameters $c_{i,\alpha}^{(k,m)}$.

From now on it will be supposed that under a coordinate transformation not the basis functions $\psi_i^{(k,m)}(r)$ but the coefficients $c_{i,\alpha}^{(k,m)}$ transform among each other. In the absence of external fields the thermodynamic potential of the system has to be invariant under any rotation of the coordinate frame. This means that in eq. (3) only invariant combinations of the coefficients $c_{i,\alpha}^{(k,m)}$ may occur. The next step is therefore to determine all the invariants set up from these coefficients.

The main difference between non-magnetic and magnetic phase transitions is that in the former case the order parameter, in powers of which the expansion of the thermodynamic potential goes, is a scalar, while in the latter case it has axial vector character. Accordingly the transformation properties of the coefficients $c_{i,\alpha}^{(k,m)}$ are given by the direct product of an irreducible representation of $G_0 \otimes R$ and the axial vector representation. This direct product can be decomposed into the irreducible representations of $G_0 \otimes R$ and the magnetization density can be expressed as linear combination of the new basis functions $\chi_i^{(k,m)}(r)$ with new coefficients. Thus eq. (2) can be written as follows

$$M(r) = \sum_{k,m,i} c'^{(k,m)}_i \chi_i^{(k,m)}(r) , \quad (4)$$

where the primed coefficients $c'^{(k,m)}_i$ are linear combinations of the unprimed ones. In what follows the primes will be dropped.

As it has been mentioned earlier, for magnetic phase transitions the time reversal R, too, has to be taken into account. Under the influence of R all the coefficients $c_i^{(k,m)}$ change sign. It corresponds to changing the sign of each internal current as well as that of the magnetization. Due to this fact there is no invariant of odd order. In the non-magnetic case the nonexistence of the third order invariants, which is necessary in order that the transition be of second order, appears as an additional criterion in selecting the representation which can describe second order phase transitions.

Constructing the even order invariants it is known that for every irreducible representation there is only one second order invariant and there is no mixed one containing coefficients belonging to different irreducible representations. Thus $\Phi_2(p, T, M(r))$ of eq. (3) can be written as

$$\Phi_2(p, T, M(r)) = \sum_{k,m} A^{(k,m)}(p, T) f^{(2)}(c_i^{(k,m)}) , \quad (5)$$

where $f^{(2)}(c_i^{(k,m)})$ is the second order invariant of the representation labelled by k and m. Above the transition point all the functions $A^{(k,m)}(p, T)$ have to be

positive and the thermodynamic potential is minimum for $c_i^{(k,m)} = 0$. Below T_c one $A^{(k,m)}(p, T)$ becomes negative continuously and the usual supposition is that it changes linearly with the temperature. This means that for a special k_0 and m_0

$$A^{(k_0,m_0)}(p, T) = a^{(k_0,m_0)} . (T - T_c)$$

with

$$a^{(k_0,m_0)} > 0 . \quad (6)$$

The minimization gives that the coefficients belonging to the representation $T^{(k_0,m_0)}$ are finite below T_c, but all the others remain zero. These coefficients can be neglected, i. e. it is possible to treat the different irreducible representations separately. It must be emphasized that this is true only after the decomposition of the direct product of the representation of the space group $G_0 \otimes R$ and the axial vector representation. If we work with the coefficients $c_{i,\alpha}^{(k,m)}$, it is possible to construct mixed invariants from coefficients with different m and α.

What we have to do now in order to determine all the possible magnetic structures for a crystal with given symmetry in the paramagnetic phase, is to take each irreducible representation of the paramagnetic space group, construct the second and fourth order invariants — the sixth order invariants play a role only in some special cases — put them into eq. (1) and minimize it with respect to the coefficients $c_i^{(k,m)}$. Inserting these values of the coefficients into eq. (2) we get the moment density in the magnetic phase.

This procedure is always feasible as all the irreducible representations of each space group are known [6]. Even if the basis functions $\Psi_i^{(k,m)}(r)$ are not known, the knowledge of their transformation properties under a coordinate transformation is enough to determine the symmetry elements that leave $M(r)$ invariant, i. e. to obtain the magnetic symmetry group. Once this group is known, it is easy to find the orientation of the moment of the individual atoms relativ to each other and to the crystallographic axes.

There are, however, two principal restrictions that have to be taken into account in this procedure. The first arises from the requirement that the magnetic structure be periodic. Lifshitz [3] has shown that in terms of group theory this can be formulated as follows : only those representations can describe periodic structures, whose antisymmetrized square does not contain common irreducible representation with the vector representation of the group G_0. As it can be shown — see reference [7] — this leads to the conclusion that only representations belonging to vectors k with rather high symmetry (vectors at the centre or at the edge of the Brillouin zone) can give periodic structures. From this it follows that if the magnetic unit cell does not coincide with the chemical one, the new lattice vector might be twice, three times or at most four times bigger than in the non-magnetic phase. If we recall, however, the fact that there are helicoidal magnetic structures, where the period of the spiral is much larger than the lattice spacing and is non-commensurable with it, we have to drop this condition. The condition for the appearance of spiral structures has been investigated by Dzyaloshinskii [8]

and here we refer only to this work without going into the details.

The other restriction for the irreducible representations has been given by Kovalev [5], who has shown that certain representations cannot give finite magnetic moment at the atomic positions. His result can be summarized as follows :

Let $\hat{G}(A)$ be the point group centered at an atom A, i. e. its elements h' transform the crystal into itself. A representation $T^{(k,m)}$ can describe magnetic moment at this atomic site only, if

$$\sum_{\hat{G}(A)} \chi^{(k,m)}(h') \neq 0 . \tag{7}$$

The character $\chi^{(k,m)}(h')$ can be expressed with the help of the character of the weighted small representation $\hat{\chi}^{(k,m)}(h)$ using the formula given by Kovalev [5]

$$\chi^{(k,m)}(h) = \sum \hat{\chi}^{(k,m)}[(h_1^s)^{-1} h h_1^s] \times$$

$$\times \exp \{ i(h^{-1} \mathbf{k}_s - \mathbf{k}_s) (\beta - \alpha_1^s) \} , \tag{8}$$

where $\mathbf{k}_1$ is a vector of the star for which the weighted small representation is known [6], $\mathbf{k}_s$ is another vector of the star, with $h_1^s \mathbf{k}_1 = \mathbf{k}_s$, where $g_1^s = \{ \alpha_1^s \mid h_1^s \}$ is an element of the group G_0, β is the position of the atom A and h is the same rotation in the original coordinate framework as h' around the atom A. The summation in eq. (8) is extended to the vectors $\mathbf{k}_s$ of the star for which $h\mathbf{k}_s$ is equivalent to $\mathbf{k}_s$.

III. Determination of simple magnetic structures. —

The actual problem in the determination of magnetic structures is not to construct all the possible structures, but to find that one that agrees with the experimental data obtained from NMR, Mössbauer or neutron diffraction measurements. The first information that these measurements can yield is the size of the magnetic unit cell compared to the chemical one. From this the vector $\mathbf{k}$ characterizing the translational behaviour can be determined. It is enough to investigate the representations belonging to this vector.

For simple magnetic structures, where from the experiment it is known that there is only a few magnetic atom per magnetic unit cell, the orientation of the moments can be calculated without knowing the irreducible representations. This method works, however, only for non-metals where the magnetic moment can be localized to the atoms.

Taking a simple structure with two magnetic atoms, let S_1^α and S_2^α (α = x, y, z) be the magnetic moment components of the first and second atoms respectively. In the neighbourhood of the transition point the thermodynamic potential Φ can be expanded directly in powers of these moment components, i. e.

$$\Phi(p, T, S_1^\alpha, S_2^\alpha) = \Phi_0(p, T) + \Phi_2(p, T, S_1^\alpha, S_2^\alpha) +$$

$$+ \Phi_4(p, T, S_1^\alpha, S_2^\alpha) + \cdots \tag{9}$$

and

$$\Phi_2(p, T, S_1^\alpha, S_2^\alpha) = \sum_i A_i(p, T) f_i^{(2)}(S_1^\alpha, S_2^\alpha) ,$$

$$\Phi_4(p, T, S_1^\alpha, S_2^\alpha) = \sum_j B_j(p, T) f_j^{(4)}(S_1^\alpha, S_2^\alpha) , \tag{10}$$

where $f_i^{(2)}$ (S_1^α, S_2^α) and $f_j^{(4)}$ (S_1^α, S_2^α) are second and fourth order invariants set up from the moment

components. Here we have already used the fact that there is no invariant of odd order.

The construction of the invariants can be done in a systematic way, knowing only the symmetry elements of the paramagnetic phase. In fourth order e. g. we take a quartic combination of the six moment components $(S_i^\alpha S_j^\beta S_k^\gamma S_l^\delta)$ where α, β, γ, δ = x, y, z and i, j, k, l = 1 or 2. Applying on it all the symmetry elements $T(g)$ and adding up these contribution, the sum

$$I = \sum_g T(g) S_i^\alpha S_j^\beta S_k^\gamma S_l^\delta \tag{11}$$

will give either zero or an invariant. Repeating now this procedure with a combination that does not appear in eq. (11), all the fourth order invariants can be obtained.

Inserting these expressions into Eq. (9, 10) and minimizing Φ with respect to the magnetic moment components supposing that at T_c one of the coefficients A_i changes sign and all the others are positive, the minimization gives at once the moment components at both atoms.

As a simple example let us investigate the magnetic structure of a few stoichiometric manganese alloys as MnPd, MnPt, MnAu, MnNi and MnRh. All these compounds crystallize in CuAuI structure and are antiferromagnetic [9] with a magnetic unit cell twice as big as the crystallographic one (see Fig. 1).
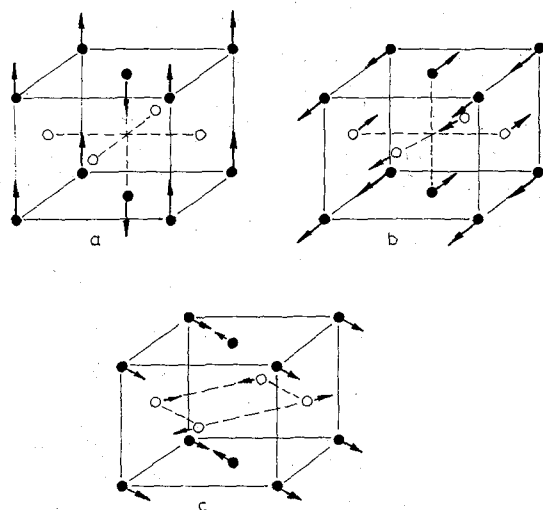

FIG. 1. — Allowed magnetic structures for CuAuI-type crystals with magnetic unit cell dimensions of $a = a_0 \sqrt{2}$ and $c = c_0$.

The translational properties of the new phase can be inferred unequivocally from the appearance of satellites in the diffraction pattern. The structure is described by the vector $\mathbf{a} = (\pi/a_0, \pi/a_0, 0)$ where a_0 is the lattice constant in the paramagnetic phase. From this it follows that $S_1 = - S_2$, where S_1 is the magnetic moment of the Mn atom at the corner of the new cell and S_2 is that of the atom in the centre of the basal plane. The problem is still the relative orientation of the moment with respect to the crystallographic axes.

Let us forget for the moment about the non-manganese atoms. Table I contains the transformation properties of the moment components under the elements of the point group. E is the unit element,

I is the inversion, C_4 is the rotation around the axis (001) through the angle $\pi/2$, u_1, u_2, u_3 and u_4 are rotations through π around the axes (100), (010), (110) and $(\bar{1}10)$, respectively, $S_4 = C_4 I$, $\sigma_h = C_4^2 I$ and $\sigma_i = u_i I$.

TABLE I

Transformation properties of the magnetic moment components in CuAuI-type lattice

E, I	C_4, S_4	C_4^2, σ_h	C_4^3, S_4^3	u_1, σ_1	u_2, σ_2	u_3, σ_3	u_4, σ_4
S_1^x	S_1^y	$-S_1^x$	$-S_1^y$	S_1^x	$-S^x$	S_1^y	$-S_1^y$
S_1^y	$-S_1^x$	$-S_1^y$	S_1^x	$-S_1^y$	S_1^y	S_1^x	$-S_1^x$
S_1^z	S_1^z	S_1^z	S_1^z	$-S_1^z$	$-S_1^z$	$-S_1^z$	$-S_1^z$

Using Table I it is easy to see that the second and fourth order invariants are as follows :

$$(S_1^x)^2 + (S_1^y)^2, \quad (S_1^z)^2,$$

$$(S_1^x)^4 + (S_1^y)^4, \quad (S_1^x)^2.(S_1^y)^2, \tag{12}$$

$$(S_1^z)^4, \quad [(S_1^x)^2 + (S_1^y)^2].(S_1^z)^2.$$

As there is no mixed second order invariant from S_1^z and S_1^x or S_1^y, the z component can be treated separately from the x and y components, i. e. the moment appearing in a second order phase transition is either along the z direction or perpendicular to it, but angles in between are not allowed. In the case when $S_1^z \neq 0$ and $S_1^x = S_1^y = 0$ we get the structure given in figure 1 a. In the other case when the moment lies in the (x, y) plane, the minimization of the free energy gives definit direction for the sublattice magnetization, namely there are two types of solutions :

1) $S_1^x \neq 0$, $S_1^y = 0$ or $S_1^x = 0$, $S_1^y \neq 0$

2) $S_1^x = \pm S_1^y$. \hfill (13)

These two possibilities are represented in figure 1 b and c. This shows that the moments has to be oriented in high symmetry directions and more complicated structures like those proposed by Kasper and Kouvel [10] for MnNi cannot arise in a second order phase transition.

Knowing now the magnetic symmetry of the crystal it is possible to investigate whether the non-manganese atoms may have magnetic moment or not. Supposing the existence of moment on these atoms they may appear together with the aligned magnetic moment of Mn provided the symmetry determined earlier does not change. The possible orientations of these moments are also given in figure 1. This symmetry argument does not say, however, anything about the relative value of the moments. The only thing we may claim is that the moment induced by the manganese atoms at the site of the non-manganese ones is small, as the effective field at these positions is small. The contribution from the first Mn neighbours is zero and only the second neighbours give non-vanishing contribution.

As a second example let us investigate the magnetic structure of Mn_3Pt [11]. The magnetic unit cell is doubled in one direction as compared to the chemical

cell of Cu_3Au-type crystals (see Fig. 2). The translational properties are described by the vector

$$\mathbf{k} = (0, 0, \pi/a),$$

where a is the lattice constant. The manganese sheets lying at a distance a are coupled antiferromagnetically, i. e. $S_1 = -S_4$, $S_2 = -S_5$ and $S_3 = -S_6$.
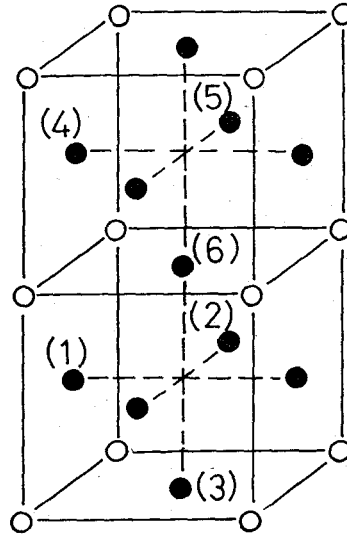

FIG. 2. — Magnetic unit cell of Mn_3Pt just below the Néel point. The Mn and Pt atoms are represented by full and empty circles respectively.

Looking for the possible magnetic structures of this system it is easy to see that the rotations and reflexions which transform the atom 3 on the basal plane into one of the positions 1, 2, 4 or 5 cannot be symmetry elements of the magnetic space group. If e. g. 3 is transformed into 1, an atom equivalent to 3 would be transformed into 4. As $S_1 = -S_4$, this transformation can be symmetry element only if $S_1 = S_4 = 0$ and $S_3 = 0$.

The remaining symmetry elements are the same as in the tetragonal CuAuI type lattice, i. e. E, C_4, u_1, u_2, u_3, u_4, I and their products. The transformation properties of the magnetic moment components under these symmetry elements are given in Table II.

It can be seen that the z component of the moment

TABLE II

Transformation properties of the magnetic moment components in Cu_3Au-type lattice

E, I	C_4, S_4	C_4^2, σ_h	C_4^3, S_4^3	u_1, σ_1	u_2, σ_2	u_3, σ_3	u_4, σ_4
S_1^x	S_2^y	$-S_1^x$	$-S_2^y$	$-S_1^x$	S_1^x	$-S_2^y$	S_2^y
S_1^y	$-S_2^x$	$-S_1^y$	S_2^x	S_1^y	$-S_1^y$	$-S_2^x$	S_2^x
S_1^z	S_2^z	S_1^z	S_2^z	S_1^z	S_1^z	S_2^z	S_2^z
S_2^x	S_1^y	$-S_2^x$	$-S_1^y$	$-S_2^x$	S_2^x	$-S_1^y$	S_1^y
S_2^y	$-S_1^x$	$-S_2^y$	S_1^x	S_2^y	$-S_2^y$	$-S_1^x$	S_1^x
S_2^z	S_1^z	S_2^z	S_1^z	S_2^z	S_2^z	S_1^z	S_1^z
S_3^x	S_3^y	$-S_3^x$	$-S_3^y$	S_3^x	$-S_3^x$	S_3^y	$-S_3^y$
S_3^y	$-S_3^x$	$-S_3^y$	S_3^x	$-S_3^y$	S_3^y	S_3^x	$-S_3^x$
S_3^z	S_3^z	S_3^z	S_3^z	$-S_3^z$	$-S_3^z$	$-S_3^z$	$-S_3^z$

is not mixed with the x and y components and therefore in the second order invariants they appear separately. This means that the moment appearing in a second order phase transition is directed either along the z axis or in the (x, y) plane but not in intermediate positions. Let us investigate now the relative orientation of the moments on the three different atoms for the case when the moments are along the z axis.

The second and fourth order invariants are as follows :

$$(S_1^z)^2 + (S_2^z)^2, \quad (S_3^z)^2$$

$$(S_1^z)^4 + (S_2^z)^4, \quad (S_1^z)^2.(S_2^z)^2, \quad (S_1^z)^3 S_2^z + S_1^z.(S_2^z)^3 ,$$

$$[(S_1^z)^2 + (S_2^z)^2].(S_3^z)^2 . \quad (14)$$

Inserting these invariants into eq. (9-10) and minimizing the thermodynamic potential, we get three types of solutions :

1) $S_1^z = S_2^z \neq 0, \quad S_3^z = 0$.

2) $S_1^z = - S_2^z \neq 0, \quad S_3^z = 0$.   (15)

3) $S_1^z = S_2^z = 0, \quad S_3^z \neq 0$.

The corresponding structures are sketched in figure 3. In the third case the magnetic symmetry of the crystal allows the existence of induced magnetic moments on the Pt sites.
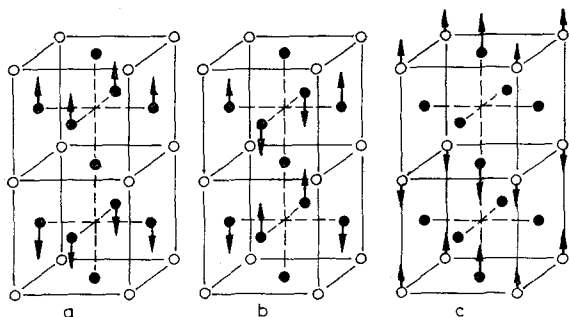

FIG. 3. — Possible magnetic structures in Cu_3Au-type lattice with magnetic unit cell doubled in the z direction and with magnetic moment lying along this axis.

IV. **Magnetic-magnetic transitions.** — Until now we have investigated the symmetry of magnetic structures arising from the paramagnetic phase. In some cases this structure does not change with decreasing temperature and the structure determined above is the ground state structure as well. In many cases, however, new phase transitions take place below the first transition point. These are often first order transitions. This theory is incapable to say anything about the new structure in such a situation. If, however, this transition from a magnetic phase to another one is of second order, the procedure applied above can be used for this transition, too [12], [13].

Let us introduce a quantity

$$M_d(r, T) = \begin{cases} 0 & \text{if } T > T_{c_2} \\ M(r, T) - M(r, T_{c_2}) & \text{if } T < T_{c_2} \end{cases}$$

where $M(r, T)$ is the actual magnetic moment density at temperature T and T_{c_2} is the second transition

temperature. This quantity can serve as small parameter in the expansion of the thermodynamic potential. The irreducible representations with the help of which $M_d(r, T)$ is written in the form of eq. (4) are that of the magnetic symmetry group of the crystal above T_{c_2}. As now the magnetic structure above this transition point is not invariant under time reversal, third order invariants may also appear. The transition, however, as we have mentioned earlier, is of second order only if there is no third order invariant. This requirement has to be checked for representations which describe transitions between magnetic phases.

Thus quite complicated magnetic structures can arise in several steps, decreasing in each step the number of symmetry elements.

V. **Concluding remarks.** — In this paper we have outlined the method how the Landau theory of second order phase transitions can be applied to determine the symmetry of the magnetic structures arising in a second order phase transition. Knowing the space group of the paramagnetic phase all the possible magnetic structures can be constructed. Using the experimental data of NMR, Mössbauer or neutron diffraction measurements the structure realized in a given system can be found. For this purpose it is not necessary to calculate all the possible structures, only those which are consistent with the translational properties inferred easily from the experiments. To summarize now the procedure the following calculation has to be done.

1) The magnetic moment density has to be written formally with the help of the irreducible representations of the space group of the paramagnetic phase with undefined coefficients $c_{i,\alpha}^{(k,m)}$ (see eq. (2)).

2) Construct the second and fourth order invariants from these coefficients and write them into the expression of the thermodynamic potential Φ (eq. (3) and (1)).

3) Minimize Φ with respect to these coefficients.

4) Inserting the obtained values for $c_{i,\alpha}^{(k,m)}$ into eq. (2), determine the symmetry of the magnetic structure.

In the case there is only a few magnetic atom in the magnetic unit cell, the procedure can be simplified as follows :

1) Assign a magnetic moment with arbitrary orientation and absolute value to each different magnetic atom.

2) Construct the second and fourth order invariants from the magnetic moment components and put them into the expression of the thermodynamic potential (eq. 9-10).

3) Minimize Φ with respect to the moment components. These components determine directly the magnetic phase.

In both cases the second and third steps, namely the construction of the invariants and the minimization of the thermodynamic potential are very important in the determination of the symmetry. We mention only, without going into details that they can be replaced by group theoritical calculations only, as it has been shown by Birman [14].

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