Application of Morse theory to the symmetry breaking in the Landau theory of second order phase transition

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Abstract :

We treat here the case of all irreps (irreducible representations) on the reals of the 32 point groups. For each point group these irreps are irreps with wave vector $k = 0$ of the corresponding space groups. Landau model of second order phase transition can be applied to those irreps with no third degree invariants : one has to look for minima of a bounded below fourth degree polynomial which is not minimum at the origin, and determine the little groups (= isotropy groups) of these minima ; they are the subgroups into which the symmetry can be broken in the transition. By an efficient strategy we reduce the study of the 153 equivalence classes of irreps to few cases (6). Moreover we do not need to study the minima of invariant polynomials, we simply apply Morse theory to find the possible little groups of minima.

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Landau theory [1] [2] of second order phase transitions in a crystal with space group G , yields a prediction for the symmetry breaking which occurs. It is given by the subgroup H (given up to a conjugation in G), little group of a minimum of a "Landau polynomial" defined on the space of a real irrep (= irreducible representation) of G with finite image. We call here "Landau polynomial" a G-invariant polynomial which has only second and fourth degree terms, is bounded below and has a maximum at the origin. We do not consider the Lifschitz condition [2,3]. A general strategy for the determination of these subgroups H could be the following.

a) List for the 230 space groups all real non-equivalent irreps with finite image, giving also their kernels and their images.

b) These irreducible images are finite subgroups of $O(m)$, the orthogonal group in m dimensions, with $1 \leq m \leq 12$. Classify them up to a conjugation in $O(m)$.

c) For each class of images compute the number of linearly independent invariant homogeneous polynomials of degree three and four. For the active representations, i.e. for those without 3rd degree invariants, determine a basis for the quartic invariants.

d) Consider all possible Landau polynomials and find the little groups of their minima.

In a) and c) we shall use the simplified approach ($\vec{k}$-equivalence technique) proposed in [4].

As an illustration of this strategy we study here all irreps of the point groups. They correspond to irreps of the space groups with wave vector $k = 0$. Since the kernel of an irrep is contained in all subgroups H of symmetry breaking, the corresponding phase transitions have no change of translational symmetry. Although the results of this paper surely exist scattered in the literature, we think that the method used here to obtain them is new and powerful. The answer to a) is contained in table 1 : 32 points groups, their 153 equivalence classes of irreps, the corresponding images and kernels. In table 1 the symbols of irreps are the same as in [5] § 11. The answer to b) is very simple and well known. Indeed, the two real one dimensional irreps are 1^+ (trivial one that we omit in table 1) and 1^- (two elements) ; the only finite subgroups of $O(2)$ which occur as images of two dimensional irreps are C_n and C_{nv} with $n = 3,4,6$. The only finite subgroups of $O(3)$ with irreducible vector representation are T , T_d , T_h , O , O_h , Y , Y_h but the last two cannot appear as homomorphic images of space groups. Total $2+6+5 = 13$ classes of images. The answer to c) is given in table 2. Only $1+4+3 = 8$ active images. Moreover the three 3-dimensional ones have the same Landau polynomials and form only one case from our point of view.

Invariant polynomials of vector representations of point groups are known [6]. However, to answer d) we do not need explicitly the Landau polynomials and we avoid the computation of their minima. Instead, we decompose the active irrep spaces into orbits and strata (see section 3 , this decomposition depends only on the image) using a systematic geometrical approach ; we then select the possible orbits of minima by application of Morse theory.

Table 4 gives the little groups of the active images and Table 5 contains all our results, listing the point groups H , subgroups of the point groups G , respected by the symmetry breaking, for the 103 active irreps of the point groups G .

These little groups H , as rightly pointed out by J.L. Birman [7], [8] are subduced subgroups for the irreps but we do not study here a strategy which could be based on J.L. Birman's criteria ; those are not completly equivalent to minimization of Landau polynomial. However we think they could be used for dévising a better strategy for points c) and d). We begun this study with Professor J.L. Birman.

I. Images of the real irreps of point groups.

Let G be a finite group.

1.) All irreducible linear representations of G on a complex vector space are equivalent to a unitary irrep ; such an irrep might be equivalent to a real representation and therefore to be an orthogonal irrep ; if the complex irrep $g \longrightarrow \Delta(g)$ is not equivalent to a real representation, then $D(g) = \Delta(g) \oplus \overline{\Delta(g)}$ is ; moreover it is irreducible on the real number field. For each real irrep we denote by $\mathcal{E}$ the real carrier space, by (x,y) the unique, up to a factor, invariant non degenerate orthogonal scalar product, and by $g \longrightarrow D(g)$ the orthogonal representation : $D(g)^T = D(g^{-1})$.

2.) The set of distinct matrices $D(g)$ of an irrep is called the image of the irrep ; it forms a group Q , isomorphic to the quotient G/K where K is the kernel of the irrep, i.e. the set of $g \in G$ such that $D(g) = I$.

3.) Given an orthogonal representation of G on $\mathcal{E}$, one should consider :
i) the orbits : $x,y \in \mathcal{E}$ are on the same orbit $\Longleftrightarrow \exists$ (there exists) $g \in G$, $y = D(g)x$.

ii) the little group = isotropy group = stabilizer G_x of each point x : it is the set of elements of G such that $D(g)x = x$. Points of the same orbits have conjugated little groups $G_{D(g)x} = gG_xg^{-1}$. Orbits which have conjugated little groups are of the same type and conversely. A stratum is the union of all orbits of the same type. We denote by $\tilde{G}$ the set of conjugation classes of subgroups of G. It carries a partial order by inclusion, up to a conjugation, of the subgroups of G, and each possible orbit or stratum is labelled by an element of $\tilde{G}$.

4.) Theorem : For every orthogonal representation of G on $\mathcal{E}$, there is a minimal little group $\in \tilde{G}$; it is the kernel K of the representation and the corresponding stratum is open dense.

Proof : $K = \bigcap_{x \in \mathcal{E}} G_x$ is the kernel of the representation ; let $\mathcal{E}^g$ be the eigen-subspace of $D(g)$ for the eigen-value 1 ; when $g \notin K$, it is a strict closed subspace of $\mathcal{E}$. The union of this finite number of strict subspaces is closed and its complement is dense ; this is just the stratum of K. We call it the "generic" stratum.

5.) If $g \longrightarrow D(g)$ is an irrep of G and α is an automorphism of G (i.e. $\alpha \in$ Aut G) then $g \longrightarrow D(\alpha(g))$ is an irrep of G. It is equivalent to $D(g)$ if α is an inner automorphism ($\alpha \in$ In Aut G) i.e. $\alpha(g) = a\, g\, a^{-1}$ with $a \in G$; hence there is an action of Out G = Aut G/In Aut G on $\hat{G}$ the set of equivalence ($\sim$) classes of irreps of G. Two non equivalent irreps on the same orbit of Out G are said to be quasi-equivalent ($\approx$).

6.) The carrier spaces $\mathcal{E}$ and $\mathcal{E}'$ of two equivalent irreps have the same composition into strata and orbits of given types. If the two irreps are only quasi-equivalent, there is a bijective map (i.e. on to one onto) between the strata and the orbits of $\mathcal{E}$ and $\mathcal{E}'$ respectively. The corresponding orbits have the same number of points but they might be not of the same type because their little groups might be not conjugated.

7.) Kernels and images of all the real irreps of point groups are listed in table 1 , where the irreps are denoted in the same way as in [5] § 11. (See also Appendix).

Table 1. - Kernels and images of the irreps of point groups.

G	Ir	Ker	Im	G	Ir	Ker	Im	G	Ir	Ker	Im	G	Ir	Ker	Im	G	Ir	Ker	Im
C_2	B	¢	1^-	C_{4h}	A^-	C_4	1^-	D_4	B_2	D_2'	1^-	D_{3h}	E^+	C_s	C_{3v}	D_{6h}	E_1^+	C_{2h}	C_{3v}
C_i,C_s	A^-	¢	1^-		B_1^+	C_{2h}	1^-		E	¢	C_{4v}		E^-	¢	C_{6v}		E_1^-	C_2	C_{6v}
C_3	$B_{1,2}$	¢	C_3		B_1^-	S_4	1^-	C_{4v}	A_2	C_4	1^-	D_{3d}	A_1^-	D_3	1^-		E_2^+	C_i	C_{6v}
C_4,S_4	B_1	C_2	1^-		$B^+_{2,3}$	C_i	C_4		B_1	C_{2v}	1^-		A_2^+	S_6	1^-		E_2^-	C_s	C_{6v}
	$B_{2,3}$	¢	C_4		$B^-_{2,3}$	C_s	C_4		B_2	C_{2v}'	1^-		A_2^-	C_{3v}	1^-	T	$B_{1,2}$	D_2	C_3
C_6	A_2	C_3	1^-	C_{6h}	A_1^-	C_6	1^-		E	¢	C_{4v}		E^+	C_i	C_{3v}		F	¢	T
	$B_{1,3}$	C_2	C_3		A_2^+	S_6	1^-	D_{2d}	A_2	S_4	1^-		E^-	¢	C_{6v}	T_h	A^-	T	1^-
	$B_{2,4}$	¢	C_6		A_2^-	C_{3h}	1^-		B_1	D_2	1^-	D_{4h}	A_1^-	D_4	1^-		$B^+_{1,2}$	D_{2h}	C_3
S_6	A^-	C_3	1^-		$B^+_{1,3}$	C_{2h}	C_3		B_2	C_{2v}'	1^-		A_2^+	C_{4h}	1^-		$B^-_{1,2}$	D_2	C_6
	$B^+_{1,2}$	C_i	C_3		$B^+_{2,4}$	C_i	C_6		E	¢	C_{4v}		A_2^-	C_{4v}	1^-		F^+	C_i	T
	$B^-_{1,2}$	¢	C_6		$B^-_{1,3}$	C_2	C_6	D_6	A_2	D_3	1^-		B_1^+	D_{2h}	1^-		F^-	¢	T_h
C_{3h}	A^-	C_3	1^-		$B^-_{2,4}$	C_s	C_6		A_3	C_6	1^-		B_1^-	D_{2d}	1^-	O,T_d	A_2	T	1^-
	$B^+_{1,2}$	C_s	C_3	D_{2h}	A_1^-	D_2	1^-		A_4	D_3'	1^-		B_2^+	D_{2h}'	1^-		E	D_2	C_{3v}
	$B^-_{1,2}$	¢	C_6		A_2^+	C_{2h}	1^-		E_1	C_2	C_{3v}		B_2^-	D_{2d}'	1^-		F_1	¢	O
D_2	A_2	C_2	1^-		A_2^-	C_{2v}	1^-		E_2	¢	C_{6v}		E^+	C_i	C_{4v}		F_2	¢	T_d
	B_1	C_2^x	1^-		B_1^+	C_{2h}^x	1^-	C_{6v}	A_2	C_{3v}	1^-		E^-	C_s	C_{4v}	O_h	A_1^-	O	1^-
	B_2	C_2^y	1^-		B_1^-	C_{2v}^x	1^-		A_3	C_6	1^-	D_{6h}	A_1^-	D_6	1^-		A_2^+	T_h	1^-
C_{2h}	A^-	C_2	1^-		B_2^+	C_{2h}^y	1^-		A_4	C_{3v}'	1^-		A_2^+	D_{3d}	1^-		A_2^-	T_d	1^-
	B^+	C_i	1^-		B_2^-	C_{2v}^y	1^-		E_1	C_2	C_{3v}		A_2^-	D_{3h}	1^-		E^+	D_{2h}	C_{3v}
	B^-	C_s	1^-	D_3,C_{3v}	A_2	C_3	1^-		E_2	¢	C_{6v}		A_3^+	C_{6h}	1^-		E^-	D_2	C_{6v}
C_{2v}	A^-	C_2	1^-		E	¢	C_{3v}	D_{3h}	A_1^-	D_3	1^-		A_3^-	C_{6v}	1^-		F_1^+	C_i	O
	B^+	C_s^x	1^-	D_4	A_2	C_4	1^-		A_2^+	C_{3h}	1^-		A_4^+	D_{3d}'	1^-		F_1^-	¢	O_h
	B^-	C_s^y	1^-		B_1	D_2	1^-		A_2^-	C_{3v}	1^-		A_4^-	D_{3h}'	1^-		F_2^+	C_i	T_d
																	F_2^-	¢	O_h

G=point group, Ir=irrep, Ker=kernel, Im=image.

$B_{i,j}=B_i\oplus B_j$, $B^{\pm}_{i,j}=B^{\pm}_i\oplus B^{\pm}_j$, dim A=dim B=1, dim E=2, dim F=3 ; $1^-=\{1,-1\}$.

II. Invariant polynomials of the real irreps of the point groups.

The representation $g \longrightarrow D(g)$ of G on $\mathcal{E}$ defines an action of G on the real valued polynomials on $\mathcal{E}$. (See [6] for the results in sections 8 and 9).

8.) A polynomial $p(x)$ on $\mathcal{E}$ is G-invariant if for all $g \in G$ and all $x \in \mathcal{E}$

$$p(D(g)x) = p(x) \quad . \tag{1}$$

Sums and products of invariant polynomials are again invariant polynomials so the set of G-invariant polynomial on $\mathcal{E}$ form a ring $\mathcal{K}^G$ which is a subring of the ring $\mathcal{K}$ of polynomials on $\mathcal{E}$.

9.) An integrity basis of $\mathcal{K}^G$ is a minimal set of homogeneous polynomials which generate it. Such a basis contains at least $m = \dim \mathcal{E}$ algebraically independent polynomials. It contains exactly m polynomials iff (=if and only if) the real representation $D(g)$ is generated by reflections, i.e. by matrices with all eigen-values 1 except one which is -1 (ref.[9]). There is some ambiguity in the choice of the polynomials θ_1 , θ_2 ,... θ_m of the integrity basis, but their degrees d_k are well defined ; we need here only to know that they satisfy the relations :

$$\Pi_{k=1}^{m} d_k = |G| \qquad \Sigma_{k=1}^{m} d_k = m + |G_1| \quad ,$$

where $|G|$ is the number of elements of G and $|G_1|$ is the number of reflections. Of course for the m dimensional irrep, $\theta_1 = \Sigma_{k=1}^{m} x_k^2$ is the lowest degree polynomial of the basis. Finally, every polynomial of $\mathcal{K}^G$ is of the form $P(\theta_1, \theta_2, \ldots, \theta_m)$ where P is an arbitrary polynomial of m variables.

Among the list of Table 1, the following images are generated by reflections :

$$1^- \ , \ C_{3v} \ , \ C_{4v} \ , \ C_{6v} \ , \ T_d \ , \ O_h \quad . \tag{2}$$

All other irrep images are invariant subgroup of index 2 of one of the image of the preceeding list, explicitly : $C_n < C_{nv}$, $T < T_d$, $O < O_h$.

Consider an image $D(G)$ generated by reflections that we denote by r_α ; let $l_a(x) = 0$, the linear homogeneous equation of the hyperplane of the reflection r_α . If H is a subgroup of G such that the restriction of D to H has an image $D(H)$ which is subgroup of index 2 of the image $D(G)$, then one proves that $\mathcal{K}^H$ is a two-dimensional module on $\mathcal{K}^G$ i.e. every H-invariant polynomial is of the form

$$P(\theta_1, \theta_2, \ldots, \theta_m) + \varphi(x) Q(\theta_1, \theta_2, \ldots, \theta_n) \tag{3}$$

where P and Q are arbitrary G-invariant polynomials and

$$\varphi(x) = \prod_{\substack{r_\alpha \in D(G) \\ r_\alpha \notin D(H)}} \ell_\alpha(x) \qquad \text{and} \quad \varphi^2 \in \mathcal{K}^G \tag{4}$$

Similarly to the table of reference [6], we give here in Table 2 the integrity basis of the ring of invariant polynomials for the real irreps of the point groups (see section 7).

Table 2 : Integrity basis of the ring of invariant polynomials for images of the real irreps of points groups :

Image	θ_1	θ_2	θ_3	φ	number of linearly independent invariants of 3^{rd},	4^{th} deg.
1^-	x_1^2				0	1
C_3	$x_1^2+x_2^2$	$x_1(x_1^2-3x_2^2)$		$x_2(3x_1^2-x_2^2)$	2	1
C_4	$x_1^2+x_2^2$	$x_1^2x_2^2$		$x_1x_2(x_1^2-x_2^2)$	0	1
C_6	$x_1^2+x_2^2$	$x_1^6-15x_1^4x_2^2+15x_1^2x_2^4-x_2^6$		$x_1x_2(3x_1^2-{}_2^2)(x_1^2-3x_2^2)$	0	1
C_{3v}	$x_1^2+x_2^2$	$x_1(x_1^2-3x_2^2)$			1	1
C_{4v}	$x_1^2+x_2^2$	$x_1^2x_2^2$			0	2
C_{6v}	$x_1^2+x_2^2$	$x_1^6-15x_1^4x_2^2+15x_1^2x_2^4-x_2^6$			0	1
T	$x_1^2+x_2^2+x_3^2$	$x_1^4+x_2^4+x_3^4$	$x_1x_2x_3$	$(x_1^2-x_2^2)(x_2^2-x_3^2)(x_3^2-x_1^2)$	1	2
T_h	$x_1^2+x_2^2+x_3^2$	$x_1^4+x_2^4+x_3^4$	$x_1^2x_2^2x_3^2$	$(x_1^2-x_2^2)(x_2^2-x_3^2)(x_3^2-x_1^2)$	0	2
T_d	$x_1^2+x_2^2+x_3^2$	$x_1^4+x_2^4+x_3^4$	$x_1x_2x_3$		1	2
O	$x_1^2+x_2^2+x_3^2$	$x_1^4+x_2^4+x_3^4$	$x_1^2x_2^2x_3^2$	$x_1x_2x_3(x_1^2-x_2^2)(x_2^2-x_3^2)(x_3^2-x_1^2)$	0	2
O_h	$x_1^2+x_2^2+x_3^2$	$x_1^4+x_2^4+x_3^4$	$x_1^2x_2^2x_3^2$		0	2

The explicit from of $\theta_2, \theta_3, \varphi$ depends on the choice of coordinates for the representation (e.g. change x_1 into x_2 and x_2 into $-x_1$) . There is also some arbitrariness in θ_2 and some times θ_3, e.g. when degree $\theta_2 = 4$, one can replace θ_2 by $\alpha\theta_1^2 + \beta\theta_2$; but the degree of the θ's are fixed. The most general invariant polynomial is $P(\theta_1, \theta_2, \theta_3) + \varphi Q(\theta_1, \theta_2, \theta_3)$ (see section 9).

Remarks : In ref.[2] (footnote near the end of § 138) the conjecture is made that there can never be more than one third degree invariant for real irreps of space groups. As this table shows for C_3 , this conjecture is wrong. It is true for complex irreps as shown in [10].

10.) We can five the stratum decomposition of each irrep. As we noted in section 6, this decomposition depends only on the image of the representation. We note that the irreps of table 2 are faithful representations of some point groups for a real irreducible component of their vector representation :

$$1^- \quad C_3 \quad C_4 \quad C_6 \quad C_{3v} \; C_{4v} \; C_{6v} \; T \quad T_h \quad T_d \quad O \quad O_h \qquad . \tag{5}$$

For the same irrep image and different groups, the little group of each stratum depends only on the kernel of the representation.

11.) All irreps of (5) have at least two strata : the origin, 0 , which is the only fixed point, and the generic stratum (see 4) which is open dense and whose little group is trivial.

The irreps $1^-, C_3, C_4, C_6$, have no other strata.

The irreps C_{nv} , $n = 3,4,6$ have another stratum, the reflectuon planes, and the corresponding little group is $Z_2(r_\alpha)$, the two element group generated by the corresponding reflexion. Note also that the two invariant polynomials θ_1 and θ_2 satisfy :

$$\Delta_3 \; : \; \theta_2^2 \leq \theta_1^3 \quad , \quad \Delta_4 \; : \; 4\theta_2 \leq \theta_1^2 \; , \quad \Delta_6 \; : \; \theta_2^2 \leq \theta_1^6 \tag{6}$$

(for Δ_4 if we had chosen $\theta_2 = x_1^4 - 6\, x_1^2 x_2^2 + x_2^4$; we would have also more generally chosen for Δ_n : $\theta_2 = \mathrm{Re}(x_1 + ix_2)^n$, then $\theta_2^2 \leq \theta_1^n = (x_1^2 + x_2^2)^n$). The equality in (6), together with $\theta_1 > 0$, defines this exceptional stratum of little group $Z_2(r)$.

There is a general method for the decomposition into strata and orbits of a representation generated by reflections ; as an example we work it out explicitly for F_1^- , the vector representation of O_h . This is the symmetry group of the cube (centered at the origin with edges parallele to the coordinate axes) and the octahedron (whose vertices are at the center of the faces of the cube). The group O_h is generated by the nine reflections through the symmetry planes of the cube ; they fall into two families : 3 symmetry planes, each containing 4 middles (m) of edges and 4 centers (n) of faces - 6 symmetry planes, each passing through 4 vertices (r) and 2 (center of face) and containing two edges - , these two types of symmetry planes correspond to two conjugate classes for the 9 reflections r_α generating O_h . These 9 symmetry planes divide the 3 dimensional space $\mathcal{E}$ into 48 triangular cones, each one of them can be considered as an orbit space. The interior of these cones is the generic stratum ; the decomposition of the cones into their geometric elements correspond to the stratum decomposition which is given in details in Table 3 .

Table 3 : Decomposition into strata and orbits of F_1^- , the vector representation of O_h.

Notation $\theta_k = \Sigma_{i=1}^{3} x_i^{2k}$ $k = 1,2,3$, $\beta = x_1 x_2 x_3$, $\alpha = (x_1^2-x_2^2)(x_2^2-x_3^2)(x_3^2-x_1^2)$
then $6\beta^2 = \theta_1^3-3\theta_1\theta_2 + 2\theta_3$, $6\alpha^2 = -18\theta_3^2 + 36\theta_3\theta_2\theta_1 - 8\theta_3\theta_1^3 + 3\theta_2^3 - 21\theta_2^2\theta_1^2 + 9\theta_2\theta_1^4 - \theta_1^6$.
Let n , r, m be respectively a center of face, a vertex and a middle of edge in the same face of the cube $-1 \leq x_i \leq 1$. The triangular cone C whose edges are the half lines containing On, Or, Om and faces Onr, Onm is an orbit space : it cuts each O_h orbit in one point.

equation, description of stratum.		nb of points in each orbit	little group	
$\alpha > 0$ $\beta^2 > 0$	inside of the cone C, generic stratum	48	$\{1\}$	symmetry plane
$\alpha = 0$ $\beta^2 > 0$	inside of face Onr of C	24	C_s	Onr
$\alpha > 0$ $\beta = 0$	inside of face Onm of C	24	C'_s	Onm
$\theta_1^3=2\theta_1\theta_2=4\theta_3 > 0$	inside of edge Om of C	12	C_{2v}	n-fold axis Om
$\theta_1^3=3\theta_1\theta_2=9\theta_3 > 0$	inside of edge Or of C	8	C_{3v}	Or
$\theta_1^3=\theta_1\theta_2=\theta_3 > 0$	inside of edge On of C	6	C_{4v}	On
$\theta_1 = \theta_2 = \theta_3 = 0$	vertex of cone C (origin)	1	O_h	

It is easy to study now the index two subgroups O , T_h , T_d ; similar study can be carried for T_d , generated by reflexions and its index two subgroup T (T is the symmetry group of the tetrahadron whose vertices are four vertices of the cube). All these results, and those obtained in section 11 are summarized in Table 4.

Table 4 : Strata of images of the Irreps of Point Groups.
For each stratum we give its dimension, its little group, the number of points of each orbit. The origin is omitted as a stratum.

Image	dim.						generic stratum
1^-	1						1 $\{1\}$ 2
C_3	2						2 $\{1\}$ 3
C_4	2						2 $\{1\}$ 4
C_6	2						2 $\{1\}$ 6
C_{3v}	2					1 $Z_2(r_a)$ 3	2 $\{1\}$ 6
C_{4v}	2				1 $Z_2(r'_a)$ 4	1 $Z_2(r'_a)$ 4	2 $\{1\}$ 8
C_{6v}	2				1 $Z_2(r'_a)$ 6	1 $Z_2(r_a)$ 6	2 $\{1\}$ 12
T	3	1 C_2 6	1 C_3^r 4				3 $\{1\}$ 12
T_h	3	1 C_{2v} 6	1 C_3^r 8	1 C_s^m 12		2 C_s 12	3 $\{1\}$ 24
T_d	3	1 C_{2v} 6	1 C_{3v}^r 4		2 C'_s 12		3 $\{1\}$ 24
O	3	1 C_4 6	1 C_3^r 8	1 C_2^m 12			3 $\{1\}$ 24
O_h	3	1 C_{4v} 6	1 C_{3v}^r 8	1 C_{2v}^m 12	2 C'_s 24	2 C_s 24	3 $\{1\}$ 48

Note that for $C_{2n,v}$, the 2n reflections are in two conjugated classes. We denote arbitrarily by $Z_2(r_a)$ and $Z_2(r'_a)$ the 2 element group generated by one reflexion of each family . For the notation C'_s , C_n^r , C_n^m , C_{nv}^r , C_{nv}^m see appendix.

III. Symmetry breaking predicted by Landau model of second order phase transitions in the irreps $k = 0$ of the crystallographic groups.

Landau theory of second order phase transitions is explained in chapter XIV of Landau and Lifschitz book on Statistical Mechanics, [2] . Although the Landau theory does not give the good critical exponents (for that it has to be quantized and reinterpreted), it seems that it predicts the good selection rules for the symmetry breaking which occurs in the transition

In order to exclude first order phase transitions, the considered irrep must have no third degree invariants. According to table 2, this excludes the irreps whose image is C_3, C_{3v}, T, T_d . The others will be called active irreps ; their list is :

Images of active irreps : $1^-, C_4, C_6, C_{4v}, C_{6v}, T_h, O, O_h$. (7)

Then we have to find the minima of a G-invariant fourth degree polynomial P which for $|x| \to \infty$ goes to $+\infty$ and is not minimum at the origin. Since the gradient dP/dx has to be G invariant at $x = 0$, $dP/dx(0) = 0$ the origin is an extremum ; moreover, at the origin the Hessian d^2P/dx^2 is invariant by the irrep of G : it has to be a multiple of the operator I and therefore P has a maximum at 0 . Hence P must have at least a G-orbit of minima at $x \neq 0$ and $|x| < \infty$. The little group H of such an orbit gives the symmetry breaking from G to H . Working first with the image of the irrep we will determine the nature of the orbit (or orbits) of minima without writing explicitly the possible P's and differentiating them. We study successively each image of the list (7).

Images $1^- C_4, C_6$. Outside the origin they have only one stratum, the generic one ; so any orbit of minima is in the generic stratum and $H = \{1\}$.

For the other irreps we will apply Morse theory ; let us recall here the main results.

12.) A smooth function f on a compact m dimensional manifold M is called a Morse function if for each of its extrema the Hessian is not degenerate (its determinant is $\neq 0$). The number k of negative eigenvalues of the Hessian is called the Morse index of the extremum (there are m-k positive eigen values). Let c_k be the number of extrema of f with Morse index k (c_0 is the number of minima, c_m that of maxima). The c_k satisfy the Morse relations :

$$n \leq m \ , \ \Sigma_{k=1}^{n} (-1)^{n-k} c_k \geq \Sigma_{k=1}^{n} (-1)^{n-k} b_k \quad , \text{ equality for } n = m \quad , \tag{8}$$

b_k is the k^{th} Betti number .

For instance if M is the m dimensional sphere $S_m, b_o = b_m = 1$ and $b_n = 0$ otherwise.

13.) If we compactify the space $\mathcal{E}$ by adding the point ∞ at infinity the G-invariant polynomial P is then a smooth function on S_m ($m = \dim \mathcal{E}$) with at least two maxima, one at 0, one at ∞ and more than one minimum (see table 4), so

$$c_0 \geq 2 \quad , \quad c_m \geq 2 \quad . \tag{9}$$

When the irrep has at least two linearly independent homogeneous fourth degree invariants (θ_1^2 is one of them), in a dense subset of the domain of its coefficients P is a Morse function. (See Appendix in [11]). In that case $(dP/dx)=0$ is a system of m polynomial equations of the third degree with a set of roots of dimension zero ; the number of real roots is at most 3^m and if we count the point ∞ :

$$c_0 + c_1 + \ldots + c_m \leq 3^m + 1 \quad . \tag{10}$$

Image C_{4v}. The Morse relations give for $m = 2$:

$$c_0 \geq 1 \quad , \quad c_1 \geq -1 + c_0 \quad , \quad c_0 - c_1 + c_2 = 2 \tag{11}$$

with equation (10) for $m = 2$ they imply

$$c_0 + (c_2 - 2) = c_1 \leq 4 \quad . \tag{12}$$

With (9) this excludes the 8 point orbits of the generic stratum ; and with the use of table 4, we find a unique solution for C_{4v} :

$$c_0 = 4 \quad , \quad c_1 = 4 \quad , \quad c_2 = 2 \quad . \tag{13}$$

This proves that, except for exceptional polynomials, the minima of the possible P's are on a four point orbit with little group $C_s = Z_2(r_a)$.

Image C_{6v}. The only fourth degree homogeneous invariant is $\theta_1^2 = (x_1^2 + x_2^2)^2$ so any fourth degree inhomogeneous invariant polynomial P is also invariant under the orthogonal group O (2) , whose orbits are the spheres centered at the origin. As explained in [2], footnote after equation 136.7 , one must consider the sixth degree invariant polynomials : they are Morse functions and (9) , (11) apply while (10) is changed into

$$c_0 + c_1 + c_2 \leq 5^2 + 1 = 26 \tag{14}$$

so

$$c_0 + c_2 - 2 = c_1 \leq 12 \quad . \tag{15}$$

This no longer implies that there are no minima of P in the generic stratum. In this rather exceptional case we have to verify it by a direct computation. Indeed, in polar coordinates ρ, ω :

$$p = \frac{P^6}{6} (\lambda + \alpha \cos 6\omega) + \beta \frac{P^4}{4} - \mu^2 P^2 \qquad \lambda > |\alpha| \quad . \tag{16}$$

Then $\frac{\partial P}{\partial \theta} = -P^6 \alpha \sin 6\omega = 0$ requires

$$\omega = k\pi/6 \qquad \text{with} \qquad 0 \leq k < 12, k \quad \text{integer} \quad . \tag{17}$$

These values of ω are the azimuths of the reflection planes ; however the 6 reflections of C_{6v} form two conjugated classes (k even and k odd), so the extrema of P occur by pair of six point orbits (2 points of the same orbit in each reflexion planes). The extrema of P satisfy

$$c_0 = 6 + 6 = c_1 \quad c_2 = 2 \qquad H = C_s = Z_2(r_a) \qquad . \tag{18}$$

Image O_h . In general P is a Morse function with the number of extrema satisfying the Morse relations :

$$c_0 \geq 1 \quad , \quad c_3 - c_2 = c_0 - c_1 \leq 1 \qquad c_3 + c_1 = c_0 + c_2 \quad . \tag{19}$$

With (9) and (10) for m = 3 we obtain :

$$c_0 \geq 2 \ , \ c_1 \geq 1 \ , \ c_2 \geq 1 \ , \ c_3 \geq 2 \qquad c_3 + c_1 = c_0 + c_2 \leq 14 \quad . \tag{20}$$

This excludes the orbits of 24 or 48 points ; since the smallest orbit has at least six points, $c_0 \geq 6$, $c_1 \geq 6$, $c_2 \geq 6$ and the only solutions are :

$$c_0 = 6 \ , \ c_1 = 12 \ , \ c_2 = 8 \ , \ c_3 = 2 \qquad H = C_{4v} \tag{21}$$

$$c_0 = 8 \ , \ c_1 = 12 \ , \ c_2 = 6 \ , \ c_3 = 2 \qquad H = C_{3v} \tag{22}$$

Images T_h, O. From table 2 we see that their fourth degree invariant polynomials P are the same that for the irrep O_h . So P is in fact invariant under a larger group than that of the image of the irrep ; when P is a Morse function this group is O_h . So the C_k are again given by (21),(22); then according to table 4, for these two irreps, each type of extrema constitute one orbit of respectively 6, 8, 12 points and the little groups of the minima are, instead of (21), (22)

$$\begin{matrix} c_0 = 6 \\ c_0 = 8 \end{matrix} \quad T_h \begin{cases} H = C_{2v} \\ H = C_3 \end{cases} \qquad O \begin{cases} H = C_4 \\ H = C_3 \end{cases} \tag{23}$$

Thus we have determined the possible orbits of minima. Each of them is characterized by a little group (up to a conjugation), subgroup of the image D(G) . When the irrep is not faithful, the inverse image in G of this subgroup is the subgroup H into which the symmetry is broken. In table 5 we list all active irreps of the point groups and the possible subgroups H of symmetry breaking.

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Table 5.- Active irreps of point groups G and subgroups H of residual symmetry in second order phase transitions.

System	G	IRREP	H
Tricl.	C_i	A^-	¢
Monoclinic	C_s	A^-	¢
	C_2	B	¢
	C_{2h}	A^-	C_2
		B^+	C_i
		B^-	C_s
Orthorhombic	C_{2v}	A^-	C_2
		B^+	C_s^x
		B^-	C_s^y
	D_2	A_2	C_2
		B_1	C_2^x
		B_2	C_2^y
	D_{2h}	A_1^-	D_2
		A_2^+	C_{2h}
		A_2^-	C_{2v}
		B_1^+	C_{2h}^x
		B_1^-	C_{2v}^x
		B_2^+	C_{2h}^y
		B_2^-	C_{2v}^y
Rhombohedral	C_{3v}	A_2	C_3
	D_3	A_2	C_3
	S_6	A^-	C_3
		$B_{1,2}^-$	¢
Rhombohedral	D_{3d}	A_1^-	D_3
		A_2^+	S_6
		A_2^-	C_{3v}
		E^-	C_2^x
			C_s^x
Tetragonal	C_4	B_1	C_2
		$B_{2,3}$	¢
	C_{4v}	A_2	C_4
		B_1	C_{2v}
		B_2	C'_{2v}
		E	C_s^x
			C_s^m
	S_4	B_1	C_2
		$B_{2,3}$	¢
	C_{4h}	A^-	C_4
		B_1^+	C_{2h}
		B_1^-	S_4
		$B_{2,3}^+$	C_i
		$B_{2,3}^-$	C_s
	D_{2d}	A_2	S_4
		B_1	D_2
		B_2	C'_{2v}
Tetragonal	D_{2d}	E	C_2^x
			C_s^m
	D_4	A_2	C_4
		B_1	D_2
		B_2	D'_2
		E	C_2^x
			C_2^m
	D_{4h}	A_1^-	D_4
		A_2^+	C_{4h}
		A_2^-	C_{4v}
		B_1^+	D_{2h}
		B_1^-	D_{2d}
		B_2^+	D'_{2h}
		B_2^-	D'_{2d}
		E^+	C_{2h}^x
			C_{2h}^m
		E^-	C_{2v}^x
			C_{2v}^m
Hexagonal	C_{3h}	A^-	C_3
		$B_{1,2}^-$	¢
	C_6	A_2	C_3
		$B_{2,4}$	¢
Hexagonal	D_{3h}	A_1^-	D_3
		A_2^+	C_{3h}
		A_2^-	C_{3v}
		E^-	C_2^x
			C_s^y
	C_{6v}	A_2	C_{3v}
		A_3	C_6
		A_4	C'_{3v}
		E_2	C_s^x
			C_s^y
	C_{6h}	A_1^-	C_6
		A_2^+	S_6
		A_2^-	C_{3h}
		$B_{1,3}^-$	C_2
		$B_{2,4}^+$	C_i
		$B_{2,4}^-$	C_s
	D_6	A_2	D_3
		A_3	C_6
		A_4	D'_3
		E_2	C_2^x
			C_2^y
	D_{6h}	A_1^-	D_6
		A_2^+	D_{3d}
Hexagonal	D_{6h}	A_2^-	D_{3h}
		A_3^+	C_{6h}
		A_3^-	C_{6v}
		A_4^+	D'_{3d}
		A_4^-	D'_{3h}
		E_1^-	D_2
			C_{2v}
		E_2^+	C_{2h}^x
			C_{2h}^y
		E_2^-	C_{2v}^x
			C_{2v}^y
Cubic	T_h	A^-	T
		$B_{1,2}^-$	¢
		F^-	C_{2v}
			C_3^r
	T_d	A_2	T
Cubic	T_d	F_1	S_4
			C_3^r
	O	A_2	T
		F_1	C_4
			C_3^r
	O_h	A_1^-	O
		A_2^+	T_h
		A_2^-	T_d
		E^-	D_{2d}
			D_4
		F_1^+	C_{4h}
			S_6^r
		F_1^-	C_{4v}
			C_{3v}^r
		F_2^-	D_{2d}
			D_3^r

Points	vertical	(0,0,1)
	m	(1,1,0)
	r	(1,1,1)

Horizontal axes		Vertical planes
D_2		C_{2v}, D'_{2d}
D'_2		C'_{2v}, D_{2d}
D_3		C_{3v}, D_{3h}, D'_{3d}
D'_3		C'_{3v}, D'_{3h}, D_{3d}

No active irreps for C_1, C_3, T. For details of notation see Appendix.

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APPENDIX.

We use Schönflies notations for the point groups : note some variations in the literature : C_i for S_2,C_{3i} for S_6, C_s instead of C_{1h} . The explicit form of invariants (e.g. table 2) depends on the position of the rotation axes and symmetry planes of these groups. They are fixed here according to the following rules. The orthonormal coordinates are x_1,x_2,x_3 . The implementation of the cubic groups is given in table 3 by a cube $-1 \leq x_i \leq 1$ of center $0(0,0,0)$; $r(1,1,1)$ is one of its vertices and $m(1,1,0)$ is the middle of an edge. For the C_n,D_n groups and those of the same family : $C_{nh},C_{nv},S_{2n},D_{nh},D_{nd}$, the n-fold rotation axis is the vertical axis Ox_3 . Let Σ and Σ' be a set of n straight lines through 0 in the horizontal plane x_1,x_2 , whose azimuths are respectively $2\pi k/n$ for Σ , $2\pi(\frac{k}{n} + \frac{1}{2})$ for Σ' with $0 \leq k < n$. Then Σ is the set of the n two fold axes of the D groups ; the vertical symmetry planes of C_{nv},D_{nk} contain Σ while those of D_{nd} contain Σ'.

In table 5 the subgroups H into which the symmetry G is broken are defined up to a conjugation by G . To precise the position of one of them, we indicate the direction of the n-fold axis by an upper index x,y,m,r for Ox_1,Ox_2,Om,Or when it is not Ox_3 . We also put a ' when the role of Σ and Σ' are exchanged.