Group Theory, and Renormalization-group theory, of Structural Phase Transitions in A-15 Systems

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Abstract

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Adviser: Professor Joseph L. Birman

The main concern of this thesis is the study of second order structural phase transitions in A-15 systems (space group O_h^3). In Chapter 2 we use the group theoretical version of the Landau Theory of Second Order Phase Transitions to find lower symmetry groups which can be achieved by order parameters of X- or R-point symmetry. Then in Chapter 3 we develop, for the first time, a general method for calculation of the Molien generating function for invariants of space groups, which we apply in Chapter 4 to the O_h^3 space group. We also find all quartic invariants for X- and R-point representations. For the six-dimensional representations *Xn, n=1,...,4 and *R4 in Chapter 6 we derive the Renormalization-group equations. We do not find any stable fixed points for these equations. Therefore we conclude that second order phase transitions, although aaowed by the Landau Theory, are not permited due to large fluctuations of the order parameter. This result seems to agree with experiment.

Acknowledgments

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CHAPTER 1

Introduction to A-15 Systems

Considerable interest in A-15 systems started in 1954 when it was found that V_3Si and Nb_3Sn, which at their room temperature crystallize in the A-15 structure, become superconductors at "high" temperatures: V_3Si at $\sim 17^{\circ}K$ and Nb_3Sn at $\sim 18^{\circ}K$. Since that time it has been found that many of the high temperature superconductors share the A-15 structure as their room temperature structure.

These superconductors are binary alloys with general chemical formula A_3B*) , A being a transition metal (usually V or Nb) and B is often a nontransition metal (usually Si, Sn, Ge, Ga, Al). Their structure (called also β-W structure) is shown at Figure 1.1 . Atoms B form a bcc lattice, whereas atoms A form three orthogonal nonintersecting chains along the cube faces; a pair of A atoms at each face are separated by half the unit cell length. The space group of A-15 systems is O_h^3-Pm3n, whose translation group N is a simple cubic so

*) They could be also pseudobinaries with B replaced by B_xC_{1-x}

that the 1st Brillouin zone is a simple cube shown in Figure 1.2 , in which high symmetry points are also shown.

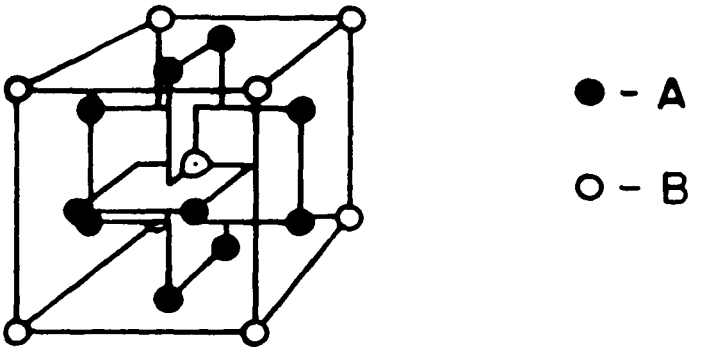

Figure 1.1

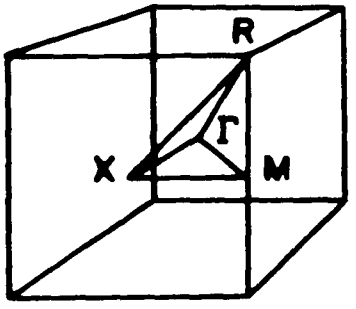

Figure 1.2

A factor group of O_h^3 with respect to N is a point group O_h :

$$O_h^3 / N = O_h \quad . \tag{1.1}$$

Coset decomposition of O_h^3 with respect to the translation group N is:

$$O_h^3 = g_1 N + g_2 N + \ldots + g_{48} N \tag{1.2}$$

where g_i is a coset representative:

$$g_i = (\phi_i | \underline{\tau}_i) \quad , \; i=1,\ldots,48 \tag{1.3}$$

and

$$g_1 = (e|\underline{0}) \quad . \tag{1.4}$$

The set of rotation-reflections ϕ_i , i=1,...,48, forms a point group O_h. With regard to fractional translations $\underline{\tau}_i$, i=1,...,48, it turns out that we can define one canonical fractional $\underline{\tau}$:

$$\underline{\tau} = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}) \tag{1.5}$$

such that all coset representatives can be written as:

$$g_i = \begin{cases} (\phi_i|\underline{0}) \ , & i=1,\ldots,24 \\ (\phi_i|\underline{\tau}) \ , & i=25,\ldots,48 \end{cases} \tag{1.6}$$

where elements ϕ_i , i=1,...,24 form a point group T_h .

For later use we list in Table 1.1 "canonical" coset representatives which we will use.

Since 1954 there has been extensive investigation of physical properties of A-15 systems. There are several good review papers on the subject[1,2]. We will just mention some of the results of these investigations.

Besides being superconducting, A-15 systems show many other anomalies and it is interesting that some of the anomalies appear even at room temperature. Such an anomaly is observed in the strong temperature dependence of the Knight-shift and magnetic susceptibility[3,4]. There is also observed anomalous behavior in the electrical resistivity[5] which rises rapidly up to about 200°K and then saturates to a relatively

TABLE 1.1

"Canonical" coset representatives of the coset decomposition of the group O_h^3 with respect to the translation group N.

$g_1=(e\|\underline{0})$	$g_{13}=(i\|\underline{0})$	$g_{25}=(c_2(1\bar{1}0)\|\underline{\tau})$	$g_{37}=(\sigma(1\bar{1}0)\|\underline{\tau})$
$g_2=(c_3(111)\|\underline{0})$	$g_{14}=(s_6^5(111)\|\underline{0})$	$g_{26}=(c_2(01\bar{1})\|\underline{\tau})$	$g_{38}=(\sigma(01\bar{1})\|\underline{\tau})$
$g_3=(c_3^2(111)\|\underline{0})$	$g_{15}=(s_6(111)\|\underline{0})$	$g_{27}=(c_2(10\bar{1})\|\underline{\tau})$	$g_{39}=(\sigma(10\bar{1})\|\underline{\tau})$
$g_4=(c_3(1\bar{1}\bar{1})\|\underline{0})$	$g_{16}=(s_6^5(1\bar{1}\bar{1})\|\underline{0})$	$g_{28}=(c_4^3(\hat{x})\|\underline{\tau})$	$g_{40}=(s_4(\hat{x})\|\underline{\tau})$
$g_5=(c_3^2(1\bar{1}\bar{1})\|\underline{0})$	$g_{17}=(s_6(1\bar{1}\bar{1})\|\underline{0})$	$g_{29}=(c_4^3(\hat{y})\|\underline{\tau})$	$g_{41}=(s_4(\hat{y})\|\underline{\tau})$
$g_6=(c_3(11\bar{1})\|\underline{0})$	$g_{18}=(s_6^5(11\bar{1})\|\underline{0})$	$g_{30}=(c_2(101)\|\underline{\tau})$	$g_{42}=(\sigma(101)\|\underline{\tau})$
$g_7=(c_3^2(11\bar{1})\|\underline{0})$	$g_{19}=(s_6(11\bar{1})\|\underline{0})$	$g_{31}=(c_2(011)\|\underline{\tau})$	$g_{43}=(\sigma(011)\|\underline{\tau})$
$g_8=(c_3(1\bar{1}1)\|\underline{0})$	$g_{20}=(s_6^5(1\bar{1}1)\|\underline{0})$	$g_{32}=(c_4(\hat{y})\|\underline{\tau})$	$g_{44}=(s_4^3(\hat{y})\|\underline{\tau})$
$g_9=(c_3^2(1\bar{1}1)\|\underline{0})$	$g_{21}=(s_6(1\bar{1}1)\|\underline{0})$	$g_{33}=(c_4(\hat{x})\|\underline{\tau})$	$g_{45}=(s_4^3(\hat{x})\|\underline{\tau})$
$g_{10}=(c_x\|\underline{0})$	$g_{22}=(\sigma_x\|\underline{0})$	$g_{34}=(c_4^3(\hat{z})\|\underline{\tau})$	$g_{46}=(s_4(\hat{z})\|\underline{\tau})$
$g_{11}=(c_y\|\underline{0})$	$g_{23}=(\sigma_y\|\underline{0})$	$g_{35}=(c_4(\hat{z})\|\underline{\tau})$	$g_{47}=(s_4^3(\hat{z})\|\underline{\tau})$
$g_{12}=(c_z\|\underline{0})$	$g_{24}=(\sigma_z\|\underline{0})$	$g_{36}=(c_2(110)\|\underline{\tau})$	$g_{48}=(\sigma(110)\|\underline{\tau})$

Note: $\bar{1}\equiv -1$

$\tau=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$

shallow linear dependence at high temperatures. Many authors have measured temperature dependence of the specific heat C_p[6], and they observed unusually high electronic contribution to the specific heat, which suggests that the electronic density of states at Fermi level must be very large. An assumed rapid increase of the density of states near the Fermi level is the basis for many models used to explain anomalies of the A-15 systems.

In some samples, at low temperatures, beside superconducting phase transition, a structural phase transition has been observed : from a cubic phase O_h^3 to a tetragonal phase. Such phase transition was first observed by Batterman and Barret[7] who observed the transition in V_3Si from a cubic phase above 21°K to a tetragonal phase with $c/a \simeq 1.0024$ below 21°K. A similar transition was observed in Nb_3Sn at 43°K, and it was found that $a/c \simeq 1.0036$. In this case the tetragonal structure has been determined as D_{4h}^9 . Although not all samples transformed, structural instability was observed in all of them. The elastic constant $(c_{11}-c_{12})$ softens with decreasing temperature (if the sample is transforming, it approaches zero at the structural transition temperature) and below a superconducting transition temperature, structural stability is reestablished.

Most of the theories have focussed their attention on the transition metal chains (the importance of the transition metal atoms is suggested by experiments in which the effect of alloying was studied).

Labbe and Friedel[8] proposed a microscopic model which assumes a one-dimensional band structure for each chain of transition metals. Furthermore, this model is purely one-dimensional since no interchain coupling is considered. In the simplest version, the Fermi level is placed close to the Γ point where one finds a singular behavior in the electronic density of states. Therefore an electronic order parameter*) would presumably have Γ symmetry. The transition is then considered as a secon order Jahn-Teller effect in which degeneracy of one-dimensional bands is lifted by the tetragonal distortion. The weak point of this theory is the neglect of interchain coupling.

On the other hand Gor'kov's model[9] assumes the Fermi level is close to the X point where there is degeneracy which is lifted by pairing of the transition metal atoms in the tetragonal phase so that electronic energy is lowered in this phase. Gor'kov considers three non-interacting chains and the interchain coupling is introduced as a perturbation.

Bhatt and McMillan[10] have worked out a Landau theory of structural phase transition based on Gor'kov's model. They consider a 9-component order parameter consisting of three charge density waves along transition metal chains coupled to

*) Anderson and Blount[12] suggested that structural phase transition must be driven by some hidden order parameter. For example, they and others suggested: electronic order parameter[13] (e.g. charge density wave, Jahn-Teller effect,...), soft optic modes[14], vacancies[15],... .

the three optic phonons, which pair transition metal atoms in the chains and which are in turn coupled to the dilatations e_{xx} , e_{yy} , e_{zz} of the unit cell.

Recently a model which assumes Fermi level close to the R point has been proposed[11]. Therefore one would assume an electronic order parameter to be of symmetry R.

In this thesis we will analyze transitions driven by an order parameter of symmetry X or R. We choose these two points in the light of Gor'kov's X-point model and the new R-point model, assuming in principle an electronically driven transition. It is not our intention to give full physical analysis of structural phase transitions in A-15 systems. We rather give analysis of possible second order phase transitions driven by an order parameter of a given symmetery: we do not make an attempt to determine which physical quantity is a relevant order parameter. This determination would have to be made on the basis of the microscopic theory which is not the concern of this thesis. We will analyze possible structural phase transitions, both by means of the Landau Theory of Second Order Phase Transitions and by Wilson's Renormalization-group approach. By comparing results obtained by these two methods and by comparing them with experiments, one may learn more about the Renormalization-group method. We focus our attention on the order parameters of symmetry X and R for the following reasons:

(a) These two points are considered separately in Gor'kov's X-point model and in the new R-point

model of the electronic structure.

(b) We are interested in the structural phase transitions involving change in the translation symmetry group.

(c) The order parameters involved are 6-dimensional, therefore the Renormalization-group approach which has not been sufficiently tested for systems involving a multicomponent (≥ 4) order parameter appears interesting.

In Chapter 2 we will give a group theoretical analysis of the possible second order structural phase transitions (Landau Theory) in A-15 structure, driven by an order parameterof symmetry X and R. Then in Chapter 6 we will give a Renormalization-group analysis for the order parameters of the same symmetry. In order to do so we will first give a general method of constructing the Molien generating function for space groups in Chapter 3. In Chapter 4 we will apply this to the X and R representations of the space group O_h^3. We will also construct quartic invariants for these representations. An introduction to the method of Chapter 6 will be given in Chapter 5.

CHAPTER 2

Landau Theory of Structural Phase Transitions in A-15 Systems.[16] Group Theoretical Approach.

The general framework of the present analysis is that of the Landau phenomenological analysis of continuous phase transitions. As this theory has been reviewed in several places,[17,18] we will give here only a brief introduction to it.

Landau has developed a theory of continuous phase transitions based on the concept of an order parameter ψ. The order parameter in Landau theory should be a quantity which changes continuously from zero in one phase to value different than zero in another phase, as temperature is changed passing a critical temperature T_c (Fig. 2.1). Also for continuous phase transitions he assumes Free Energy Φ to be a <u>continuous</u> function of an order parameter and other thermodynamic variables T, P, ... However, the order parameter is itself a function of thermodynamic variables. It is determined from a minimization of Free Energy $\Phi(T, P, \ldots ; \psi)$ with respect to ψ. Furthermore, since in the neighborhood of the critical

point the order parameter is small, we can expand the Free Energy in a power series of the order parameter as:

$$\Phi(T,P,\ldots;\ )=\Phi_0+\alpha\psi+A\psi^2+C\psi^3+B\psi^4+\ldots \qquad (2.1)$$

where Φ_0, α, A, B, ... are analytic functions of T, P, ... We will assume here that a higher symmetry phase corresponds to a disordered system and $T>T_c$. Therefore for $T>T_c$ we want

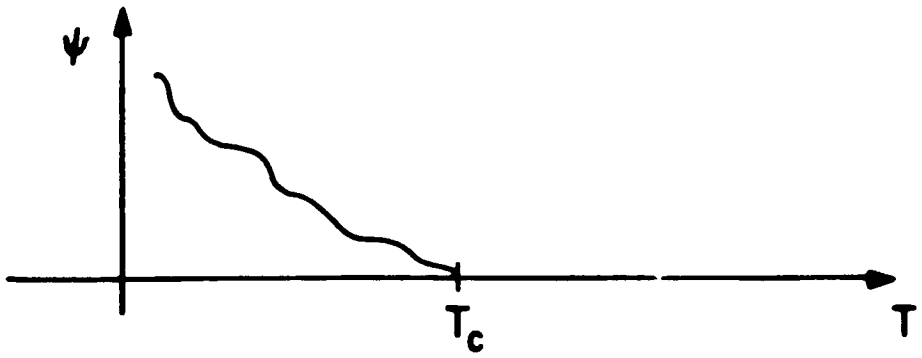

Figure 2.1

$\psi=0$ to be a minimum. That in turn implies $\alpha=0$ and $A>0$. Since $\alpha=0$ for $T>T_c$ and is an analytic function of T, P, ... we conclude $\alpha=0$ everywhere (later we will also justify this conclusion gy symmetry arguments). Therefore for $T<T_c$, $\psi=0$ is still an extremum, however if do not want it to be a minimum then we must assume $A<0$ for $T<T_c$. Thus we conclude that A may be written as

$$A(T,P,\ldots)=a(P,\ldots)(T-T_c) \qquad (2.2)$$

where $T_c=T_c(P,\ldots)$ is a transition temperature. Therefore we conclude that at the critical temperature $A=0$. Also for $\psi=0$ to be a <u>minimum</u> we need $C=0$ and $B>0$ at the transition temperature. Since we are interested in the systems having a critical line, not a point, condition $C=0$ must be identically sat-

isfied (i.e. by symmetry). Since the coefficient B is greater than zero at $T=T_c$ we take it to be effectively independent of T. Therefore Φ is given as:

$$\Phi=\Phi_0+a(P,...)(T-T_c)\psi^2+B(P,...)\psi^4. \qquad (2.3)$$

Then the low symmetry value of the order parameter obtained by the minimization of (2.3) is given by:

$$\psi^2=\frac{a}{2B}(T_c-T) \quad . \qquad (2.4)$$

From Eqs. 2.3 and 2.4 it is easy to conclude that entropy is continuous at $T=T_c$, whereas specific heat C_p exhibits discontinuity.

We have just analyzed a second order transition with some definite symmetry change which we have assumed possible. This theory however does not tell us whether such symmetry change could arise via a second order phase transition. Next we will address this question.

We will consider a phase transition involving change of crystal symmetry. An important role in this theory is played by the density function $\rho(r)$ which represents a probability that an atom of the crystal will be found around r. Therefore the symmetry of the crystal is a group of all transformations which leave $\rho(r)$ invariant. A typical example is a linear chain of identical atoms whose density function at $T\geq T_c$ and $T<T_c$ we represent on Fig. 2.2 where the symmetry change is reflected in a doubling of the unit cell.

Let G_0 be a symmetry group at the transition point. Then function $\rho(r)$ could be expanded at any temperature as:

$$\rho(r)=\rho_0(r) + \delta\rho \quad , \qquad (2.5)$$

where $\rho_0(r)$ is invariant under G_0 and $\delta\rho$ is conventionally given by the expansion

$$\delta\rho = \sum_n{}' \sum_i \psi_i^{(n)} \phi_i^{(n)}(r) \quad , \tag{2.6}$$

where: $\sum_n{}'$ is a sum over all ireducible representations of G_0, except the identity representation; $\phi_i^{(n)}(r)$ is the i^{th} basis function of the n^{th} irreducible representation $\Gamma^{(n)}$ of G_0; $\psi_i^{(n)}$ are arbitrary parameters. Also we must remark that since

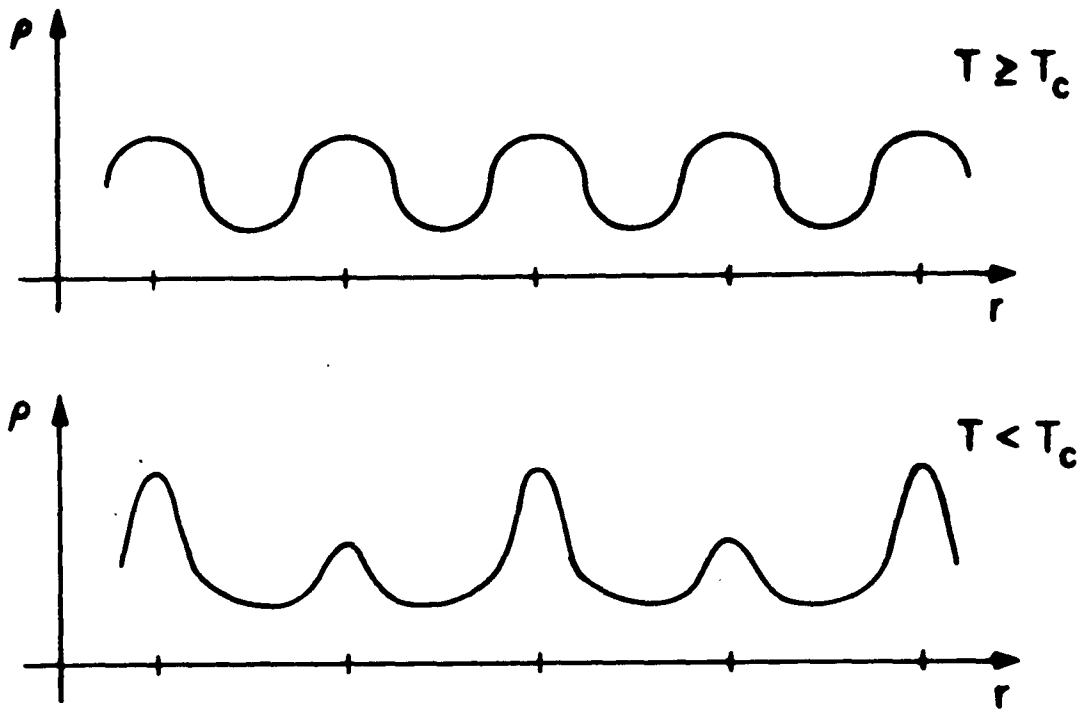

Figure 2.2

ρ is real we will consider only physically irreducible representations in expansion (2.6).

Since the parameters $\psi_i^{(n)}$ determine the actual symmetry group we will take them as order parameters. Any symm-

etry operation gGG_0 on ρ is equivalent to the linear transformation on the set $\psi_i^{(n)}$. So we can consider $\psi_i^{(n)}$ to transform under G_0 as:

$$G_0:\psi_i^{(n)}\rightarrow\sum_j\Gamma_{ji}^{(n)}\psi_j^{(n)} \quad . \tag{2.7}$$

Now we can expand the Free Energy as:

$$\Phi=\Phi_0+\Phi_1+\Phi_2+\Phi_3+\Phi_4+\ldots \quad , \tag{2.8}$$

where Φ_i is of i^{th} degree in set $\psi_i^{(n)}$. However, since Φ should be invariant under G_0, every Φ_i should be invariant under G_0. This automatically rules out Φ_1. Furthermore, for all physically irreducible representations there is only one quadratic invariant:

$$\Phi_2=\sum_n{}' A^{(n)}\sum_i(\psi_i^{(n)})^2 \quad . \tag{2.9}$$

At $T=T_c$ the symmetry is G_0 and thus all $\psi_i^{(n)}$ are zero and that value must corespond to a minimum of Φ. This in turn implies that all $A^{(n)}>0$ at $T=T_c$. But, since $A^{(n)}$ is an analytic function,in the neighborhood of $T=T_c$ $A^{(n)}$ would also be greater than zero and thus $\psi_i^{(n)}=0$ would always be a minimum and no symmetry change would occur. Therefore at least one $A^{(n)}$ should change sign at $T=T_c$. That particular $A^{(n)}$ will be kept in the expansion with $\psi_i^{(n)}$ taken to belong to that particular representation. Thus we take:

$$\delta\rho=\sum_i\psi_i\phi_i(r) \tag{2.10}$$

and

$$\Phi=\Phi_0+A\sum_i\psi_i^2+\sum_j C_j I_j^3+\sum_j B_j I_j^4+\ldots \quad , \tag{2.11}$$

where I_j^m is the j^{th} independent invariant of the m^{th} degree

in the set $\{\psi_i\}$. Then, considerin Φ at $T=T_c$, we conclude that all C_j must be zero at $T=T_c$ and therefore, since we are interested in the system having a critical line, that term must be identically zero (i.e. corresponding representation Γ of G_0 should not have a cubic invariant), and the coefficients B_j must be such that the expansion tends to $+\infty$ as $\sum\psi_i^2 \to +\infty$. This B_j must be such that the expansion tends to $+\infty$ as $\sum_i \psi_i^2 \to +\infty$. is often called the Landau condition.

In order to rule out possible spatial inhomogeneity of an order parameter, which would give rise to a term of the form $(\psi_i \partial\psi_j/\partial r_\alpha - \psi_j \partial\psi_i/\partial r_\alpha)$ we have to impose a condition on representation , namely that it must not contain such an invariant. This condition is called the Lifshitz condition. However, there is experimental evidence that some systems develop below a critical temperature a spatially inhomogeneous order parameter, so that it is not certain whether the Lifshitz condition really must be satisfied for the phase transition to be of the second order.

The next step is to determine a low symmetry phase. This is conventionally done by determining a set $\{\psi_i\}$ which minimizes the Free Energy Φ given by

$$\Phi=\Phi_0+A\sum_i\psi_i^2+\sum_j B_j I_j^4 \quad . \qquad (2.12)$$

Then with $\{\psi_i\}$ so obtained one goes back to $\delta\rho$ and determines a low symmetry group G_1 as one which leaves $\delta\rho$ invariant.

This theory has been simplified into several group theoretical algorithms.[19] These algorithms have the merit of

reducing the tedious minimization associated with the usual method and have been applied to investigate symmetry change in phase transitions for several systems,[20] including some with magnetic symmetry.[21]

These algorithms are:

(1) The Landau condition, given in the group theoretical language is:

$$\{\Gamma^3\} \not\subset \Gamma^{1+} \text{ of } G_0 \quad . \tag{2.13}$$

That is: the symmetrized cube of Γ shall not contain the identity representation of G_0.

(2) The Lifshitz condition, given as:

$$(\Gamma^2) \not\subset \Gamma^{v} \text{ of } G_0 \quad . \tag{2.14}$$

That is: the antisymmetrized square of Γ shall not contain the vector representation of G_0.

(3) The subduction criterion: G_1 is an allowed subgroup of G_0 if

$$\Gamma \text{ of } G_0 \downarrow \Gamma^{1+} \text{ of } G_1 \quad , \tag{2.15}$$

where $\downarrow$ means subduces. This criterion has been introduced by J.L.Birman[19] in order to avoid minimization of the Free Energy which is especially difficult for many component order parameters. It is clear that every group G_1 obtained by minimization will satisfy this condition. However, the converse has not as yet been proven.

(4) The chain subduction criterion: if G_1' is a subgroup of G_1 and if G_1 is a subgroup of G_0, and if Γ of $G_0 \downarrow \Gamma^{1+}$ of G_1 (c times) and Γ of $G_0 \downarrow \Gamma^{1+}$ of G_1' (d times, c and d positive integers), then G_1' is allowed as well as G_1 if d is greater

than c. Otherwise G_1' is not allowed. This criterion is a direct consequence of the assumption that the converse in the previous criterion holds: assume that c=d then G_1 and G_1' in the minimization procedure will correspond to the identical minimum of Φ and therefore to identical $\delta\rho$, however, by assumption , the highest symmetry group which leaves $\delta\rho$ invariant is a symmetry group of the system and thus G_1 but not G_1' is a new symmetry group.

We have used all these criteria in our investigation.

In the A-15 structure the translation group is primitive so that the first Brillouin zone is a simple cube. The group theory has been given by Gorzkowski, Mattheiss and others,[22] and the irreducible representations are known. Since there are two molecules/cell there are quite a few available representations.

The particular points in the Brillouin zone at which attention can be focussed are Γ, X and R. These are the points where it would appear that the most likely order parameter symmetries should originate.

The point Γ in the zone is the focus of attention in the Labbe-Friedel-Barišić[23] model of electronic structure. Possible order parameters of symmetry Γ (vector representations of the point group O_h) have been analyzed previously. Anderson and Blount[12] showed that elastic strain could not be an order parameter in the cubic structure for continuous cubic-tetragonal symmetry change. Possible optic mode order parameters

were investigated by Birman[14] and compatible subgroups and order parameters were given.

The point X is of interest because of recent work by Gor'kov[9] who places the Fermi level in A-15 alloys near X. We have examined representations *Xn, n=1,2,3,4.[28] These are all two-dimensional ray representations of the point group D_{4h} yielding six-dimensional irreducible representations of O_h^3. We find that *X3 and *X4 satisfy both Landau and Lifshitz criteria. Thus these are both compatible representations for a second order phase transition. Note these representations are called X_1, X_3 by Gor'kov and he does not employ them in his theory. The predicted (sub)space groups are given in Table 2.1, for cell doubling in one direction, and in Table 2.2 for cell doubling in two directions. In both tables the extreme right hand column gives the effect of employing the chain subduction criterion. Therefore the subgroups listed, which emanate from representations *X3 and *X4, are to be understood as achievable by second order phase transitions in the strict sense.

On the other hand we find that the representations *X1 and *X2 satisfy Landau but not Lifshitz criterion. Thus strictly speaking, these representations give rise to first order transitions. But the Lifshitz criterion has had a somewhat ambiguous history[24] and in our opinion it is not yet settled whether in fact this condition needs to be obeyed for a transition to be second order. The group theory results are given in Tables 2.1 and 2.2 for representations *X1 and *X2.

TABLE 2.1

Phase Transitions in O_h^3 Based on *Xm , m=1,2,3,4. Phases Resulting from Doubling in One Direction

Irrep.	c	Subgroups after subduction	Allowed subgroups
*X1	2	C_{2v}^1, C_2^1, C_s^1, C_1^1	C_{2v}^1
	1	D_{2h}^1, D_{2d}^5, D_2^1, S_4^1, C_{2h}^1, C_i^1	D_{2h}^1, D_{2d}^5
*X2	2	C_{2v}^3, C_2^1, C_s^2, C_1^1	C_{2v}^3
	1	D_{2h}^3, D_{2d}^6, D_2^1, S_4^1, $C_{2h}^{1,4}$, C_{2v}^4, C_s^1, C_i^1	D_{2h}^3, D_{2d}^6
*X3	2	D_2^2, $C_2^{1,2}$, C_1^1	D_2^2
and	1	D_{2h}^5, $D_4^{3,7}$, $C_4^{2,4}$, $C_{2v}^{1,2,4}$, $C_{2h}^{1,2,4}$, $C_s^{1,2}$, C_i^1	D_{2h}^5, $D_4^{3,7}$
*X4			

TABLE 2.2

Phase Transitions in O_h^3 Based on *$\underline{X}$m , m=1,2,3,4. Phases Resulting from Doubling in Two Directions

Irrep.	c	Subgroups after subduction	Allowed subgroups
*$\underline{X}$1	4	C_s^1, C_1^1	C_s^1
	3	C_{2v}^1, C_2^1	C_{2v}^1
	2	D_{2h}^1, C_{2v}^4, D_2^1, C_{2h}^1, C_s^2, C_i^1	D_{2h}^4, C_{2v}^4
	1	D_{4h}^9, $D_{2h}^{3,5}$, C_{4v}^7, C_{4h}^2, D_4^5, $C_{2v}^{2,3}$, S_4^1, C_4^3, D_2^2, $C_{2h}^{2,4}$, C_2^2	D_{4h}^9, $D_{2h}^{3,5}$
*$\underline{X}$2	4	C_s^2, C_1^1	C_s^2
	3	C_{2v}^6, C_2^1	C_{2v}^6
	2	D_{2h}^4, $C_{2v}^{3,8}$, D_2^1, C_{2h}^4, C_i^1	D_{2h}^4, C_{2v}^3
	1	D_{4h}^{11}, $D_{2h}^{3,7,8}$, $D_{2d}^{2,7}$, C_{4v}^8, C_{4h}^4, D_4^5, $C_{2v}^{4,5,7}$, S_4^1, C_4^3, D_2^2, $C_{2h}^{1,5}$, C_2^2, C_s^1	D_{4h}^{11}, $D_{2h}^{3,7,8}$
*$\underline{X}$3	4	D_2^3, $C_2^{1,2}$, C_1^1	D_2^3
and	2	$D_{2h}^{9,11,13}$, D_4^6, $C_{2h}^{1,2,4,5}$, S_4^1, C_4^3, $C_{2v}^{1,2,4,5,7,8}$, $C_s^{1,2}$, C_i^1	$D_{2h}^{9,11,13}$, D_4^6, S_4^1
*$\underline{X}$4	1	$D_{4h}^{13,15}$, $D_{2h}^{5,7,8}$, $D_{2d}^{4,5,7}$, $C_{4v}^{7,8}$, $C_{4h}^{2,4}$, D_2^2, $C_{2v}^{3,6}$	$D_{4h}^{13,15}$, $D_{2h}^{5,7,8}$

The transitions there listed may be regarded as first order "in principle", but perhaps weakly so. Representations *X1 and *X2 are called X_2 and X_4 by Gor'kov and they are employed in his theory.

Note that Tables 2.1 and 2.2 give space groups which arise from a doubling of the fundamental translation in one, or two directions respectively.

The point R in the Brillouin zone has recently been investigated in a new model for electronic and lattice properties of A-15 compounds.[11] Interest in the states around that point has arisen in part because recent energy band calculations[25] show the Fermi level in several A-15 compounds (V_3Si); Nb_3Sn, *inter alia*) to be near R. States there may then be eligible to participate as "order parameters".

We have investigated representations *Rm, m=1,2,3,4. (we use here the notation of Miller and Love[28]). But representations *R2 and *R3 are complx conjugates so that we consider the "physically irreducible" representations: *R1, *R'2 *R2⊕*R3 and *R4.

We find that *R1 and *R'2 satisfy both Landau and Lifshitz conditions. The resultant lower symmetry phases with doubling of unit cell in all three directions which can arise are given in Table 2.3. These are to be understood as being "strictly" second order transitions.

We find that *R4 satisfies Landau but not Lifshitz condition. The resulting lower symmetry phases which can arise with a doubling of the unit cell in all three directions

TABLE 2.3

Phase Transitions in O_h^3 Based on *Rm , m=1,'2,4. Phases Resulting from Doubling in All Directions

Irrep.	c	Subgroups after subduction	Allowed subgroups
*R1	2	$T^{1,4}$, C_3^4, D_2^{1-4}, $C_2^{1,2}$, C_1^1	$T^{1,4}$, $D_2^{2,3}$
	1	$T_h^{1,2,6}$, $O^{6,7}$, D_3^7, C_{3i}^2, D_{2h}^{1-16}, $D_4^{3,4,7,8}$, $C_{2h}^{1,2,4,5}$, C_{2v}^{1-10}, $C_4^{2,4}$, $C_s^{1,2}$, C_i^1	$T_h^{1,2,6}$, $O^{6,7}$, $D_{2h}^{3-14,16}$, $D_4^{3,4,7}$
*R'2	4	D_2^{1-4}, $C_2^{1,2}$, C_1^1	D_2^{1-4}
	2	D_{2h}^{1-16}, $D_4^{3,4,7,8}$, $C_4^{2,4}$, C_{2v}^{1-10}, $C_{2h}^{1,2,4,5}$, $C_s^{1,2}$, C_i^1	D_{2h}^{1-16}, $D_4^{3,4,7,8}$
*R4	6	C_1^1	C_1^1
	4	$C_2^{1,2}$	$C_2^{1,2}$
	3	$C_s^{1,2}$, C_i^1	$C_s^{1,2}$, C_i^1
	2	S_4^1, C_{2v}^{1-10}, $C_{2h}^{1,2,4,5}$, D_2^{1-4}, C_3^4	↔ same
	1	D_3^7, C_{3i}^2, D_{2d}^{5-8}, D_{2h}^{1-16}, $D_4^{3,4,7,8}$, $C_4^{2,4}$	} ↔ same

are also set forth in Table 2.3, and may be considered "weakly" first order according to the rationale given above.

As far as we have been able to determine there exists two definitive structure analyses with wich we ca compare our results. These are determinations of lower symmetry space groups for alloys originally in the A-15 structure.

The first is:

$$Nb_3Sn - D_{4h}^9 \quad , \tag{2.16}$$

a (weak) first order transition with no cell multiplicity.[26] Since there is no cell (translational) multiplicity, the relevant order parameter here has been taken as belonging to representation Γ^{12+}, which would, of course, produce a first order transition.[9,12] Recently,[10] a model based on the use of a charge-density-wave(CDW) with electronic (CDW) order parameter symmetry $*\underline{X}2$ has been put forth for Nb_3Sn based on Gor'kov's X-point model. The CDW model requires a coupling of the order parameter Γ^{12+} to the CDW in the Ginzburg-Landau type Free Energy.

The second case is:

$$Nb_3Si - C_{4h}^4 \quad , \tag{2.17}$$

doubling in x and y directions;[27] thermodynamic order not determined. According to our work, the transition $O_h^3 \rightarrow C_{4h}^4$ with doubling in two directions can occur only for an order parameter belonging to $*\underline{X}2$ with the additional assumption that the chain criterion is not applicable. The transition should be weakly first order. This follows from Table 2.2 and the fail-

ure of *X2 to satisfy the Lifshitz and chain criteria. In Ref. 27 no information regarding the order of this transition was given: we suggest it may be "weakly" first order.

CHAPTER 3

Calculation of the Molien Generating Function for Invariants of Space Groups[29,30]

There are various physical problems for which it is of importance to determine polynomial invariants of a group G. The first step in the explicit determination of such invariants is to obtain the number of invariants of given degree. This can be accomplished by use of the Molwen function,[31] for representation Γ of group G (definition of the Molien generating function will be given below). Actual construction of the invariants is a separate step which can be accomplished by use of projection operators or an equivalent algebraic technique. Knowledge of the structure of the Molien function provides a useful guide for determination of the integrity basis of the ring of invariants.

If one is concerned with a phase transition in a crystal, one may have focused attention upon some multicomponent order parameter $(x_1,\ldots,x_l)$, where x_j are vectors in a Hilbert space, such that under action of elements g in G

$$g: (x_1,\ldots,x_l)\rightarrow\Gamma(g) \qquad (3.1)$$

where Γ is an l-dimensional irreducible representation of G. For the present we suppress all inddices relating to the representation. Then, the first step in modern renormalization-group calculations requires construction of the Hamiltonian for the system based on these order parameters.[32] The Hamiltonian is taken as a power series in the set $(x_1,\ldots,x_l) \equiv(x)$

$$H(x)=H^{(0)}(x)+H^{(1)}(x)+\ldots+H^{(s)}(x)+\ldots \quad , \qquad (3.2)$$

where the terms in $H^{(s)}(x)$ will be a sum of the independent polynomial invariants, each homogeneous of degree s in the set (x). This so-called Landau-Ginzburg-Wilson expression is usually truncated at s=4 or 6, but future work may require considering terms of higher degree, or the entire function H(x).

Work in the framework of phenomenological (Landau) theory of phase transitions in crystals[33] requires knowledge of the basic invariants (integrity basis), and in some forms of the theory, one needs expansions of the Gibbs free energy F(x) in a power series like (3.2).[34]

A third example is the calculation of selection rules for higher order optical processes such as multiphonon infrared or Raman processes.

The Molien function for a finite group G is the generating function for the multiplicity c_{nl} with which the trivial or identity representation Γ^{1+} is contained in the

symmetrized n^{th} power of a representation Γ of G. The Molien function is also the formal power series

$$M(\Gamma,G;z)=\sum_{n=0}^{\infty} c_{n1} z^n \quad . \tag{3.3}$$

By definition $c_{n0}\equiv 1$. The usual form for the generating function is

$$M(\Gamma,G;z)=\frac{1}{|G|}\sum_{g}\frac{1}{\det\{1-z\Gamma(g)\}} \quad , \tag{3.4}$$

where the sum is over all elements g in the group G, $|G|$ is the order of G.

It may be helpful in the interpretation of (3.3), (3.4) to recall that if, in the 1-dimensional representation Γ of G we diagonalize the one matrix $\Gamma(\bar{g})$ for element $\bar{g}$ and find its l eigenvalues

$$\mathrm{diag}\Gamma(\bar{g})=(\bar{\omega}_1,\ldots,\bar{\omega}_1) \quad , \tag{3.5}$$

then we can construct the partial Molien function for element $\bar{g}$ in the representation Γ:

$$m(\Gamma,\bar{g};z)\equiv\prod_{i=1}^{l}(1-z\bar{\omega}_i)^{-1} \tag{3.6}$$

and

$$M(\Gamma,G;z)=\frac{1}{|G|}\sum_{g} m(\Gamma,g;z) \quad . \tag{3.7}$$

Also, since the partial molien function is a class function,

$$M(\Gamma,G;z)=\frac{1}{|G|}\sum_{k} c_k m(\Gamma,C_k;z) \quad , \tag{3.8}$$

where the sum is over all classes C_k in the group G, and c_k is the order of class C_k.

In actual application, the forms 3.4, 3.6 have the disadvantage of requiring diagonalization of all the Γ.

First we will give two equivalent presentations for the Molien function, only requiring the characters

$$\chi(g)=\mathrm{Tr}\Gamma(g) \quad , \tag{3.9}$$

which are more readily available. This should facilitate applications, especially to crystal space groups.

From the character system for the symmetrized n^{th} power of representation Γ we can find the c_{nl}. Let $\chi_{(n)}(g)$ be the character of g in the symmetrized n^{th} power of Γ; then, since all characters of Γ^{1+} are 1,

$$c_{nl}=|G|^{-1}\sum_{g}\chi_{(n)}(g) \quad . \tag{3.10}$$

A closed, but chumbersome expression exists[35] for $\chi_{(n)}(g)$:

$$\chi_{(n)}(g)=\sum_{\kappa_1,\ldots,\kappa_n}\frac{\chi^{\kappa_1}(g)\ldots\chi^{\kappa_n}(g^n)}{1^{\kappa_1}\kappa_1!\ldots n^{\kappa_n}\kappa_n!} \quad , \tag{3.11}$$

with

$$\sum_{l=1}^{n} l\kappa_l=n \tag{3.12}$$

and κ_l zero or a positive integer. The objective of this section is to rewrite $\chi_{(n)}$ in terms of a simpler generating function and thereby also c_{nl}.

First we include the condition 3.12 by incorporating it as a Kronecker delta in 3.11, and extending multiple sums on $\kappa_1,\ldots,\kappa_n$ to infinity:

$$\chi_{(n)}(g)=\sum_{\kappa_1,\ldots,\kappa_n}\delta_{n,\Sigma l\kappa_l}\frac{\chi^{\kappa_1}(g)\ldots\chi^{\kappa_n}(g^n)}{1^{\kappa_1}\kappa_1!\ldots n^{\kappa_n}\kappa_n!} \quad . \tag{3.13}$$

Next we use an integral representation of the delta

$$\delta_{p,0}=\mathrm{Res}\frac{1}{z^{p+1}}=\frac{1}{2\pi i}\oint_c\frac{dz}{z^{p+1}} \quad , \tag{3.14}$$

with p integer, where c is a closed contour around z=0 and

Res means "residue". Substituting 3.14 into 3.13 we obtain

$$\chi_{(n)}(g)=\frac{1}{2\pi i}\oint_c \frac{dz}{z^{n+1}}\prod_{l=1}^{n}\sum_{\kappa_l=0}\frac{z^{l\kappa_l}\chi^{\kappa_l}(g^l)}{l^{\kappa_l}\kappa_l!} \quad . \tag{3.15}$$

We also used

$$\sum_{l=1}^{n} z^{l\kappa_l}=z^{\Sigma l\kappa_l} \quad . \tag{3.16}$$

Now Eq. 3.15 can be rearranged to give

$$\chi_{(n)}(g)=\frac{1}{2\pi i}\oint_c \frac{dz}{z^{n+1}}\prod_{l=1}^{n}\sum_{\kappa_l=0}^{\infty}\left[\frac{z^l\chi(g^l)}{l}\right]^{\kappa_l}\frac{1}{\kappa_l!} \quad , \tag{3.17}$$

which can now be recognized as follows:

$$\chi_{(n)}(g)=\frac{1}{2\pi i}\oint_c \frac{dz}{z^{n+1}}\prod_{l=1}^{n}\exp\frac{z^l\chi(g^l)}{l}=$$

$$=\frac{1}{n!}\frac{d^n}{dz^n}\exp\left\{\sum_{l=1}^{n}\frac{z^l\chi(g^l)}{l}\right\}\Bigg|_{z=0} \quad . \tag{3.18}$$

We may now formally extend the sum upon l to ∞. This sum is convergent since we may take $|z|<1$; also for finite groups the characters of powers of g are periodic (e.g., if p is the smallest positive integer such that $g^p=e$, then $\chi(g^{l+p})=\chi(g^l)$):

$$\chi_{(n)}(g)=\frac{1}{n!}\frac{d^n}{dz^n}\left\{\exp\sum_{l=1}^{\infty}\frac{z^l\chi(g^l)}{l}\right\}\Bigg|_{z=0} \quad , \tag{3.19}$$

which is the n^{th} term in the Taylor expansion about z=0 of the function inside the curly brackets. Hence

$$\exp\sum_{l=1}^{\infty}\frac{z^l\chi(g^l)}{l}=\sum_{n=0}^{\infty}\chi_{(n)}(g)z^n \quad , \tag{3.20}$$

where $\chi_{(0)}(g)\equiv 1$ by definition.

Recalling Eq. 3.10 we have

$$M(\Gamma,G;z)=|G|^{-1}\sum_g \exp\sum_{l=1}^{\infty}\frac{z^l\chi(g^l)}{l}=\sum_{n=0}^{\infty}c_{nl}z^n \quad . \qquad (3.21)$$

This is our first expression for the Molien function in terms of a generating function which depends only on the character system of the representation.

To verify the connection with the usual form of the Molien function, we observe

$$\chi(g^l)=Tr\{\Gamma(g^l)\}=Tr\{\Gamma(g)^l\} \quad . \qquad (3.22)$$

Then the exponential function becomes

$$\exp\{Tr\sum_{l=1}^{\infty}\frac{z^l\Gamma(g)^l}{l}\}=\det\exp\sum_{l=1}^{\infty}\frac{z\Gamma(g)^l}{l} \quad . \qquad (3.23)$$

But for $|z|<1$

$$-\ln\{1-z\Gamma(g)\}=\sum_{l=1}^{\infty}\frac{\{z\Gamma(g)\}^l}{l} \quad , \qquad (3.24)$$

and, substituting back into Eq. 3.23, we have

$$\det\exp\{-\ln(1-z\Gamma(g))\}=\det\{(1-z\Gamma(g))^{-1}\}=$$
$$=\{\det(1-z\ (g))\}^{-1} \quad . \qquad (3.25)$$

All that now remains is to average this expression over the group by multiplying by $|G|^{-1}$ and summing on g to recover Eq. 3.4.

Let us return to (3.6), (3.7). In these equations the eigenvalues of $\Gamma(g)$ appear. If G is a finite group, then, as previously remarked, every element has finite period p: $g^p=e$. Of course, $p\leq|G|$. Consequently, $\Gamma(g^p)=\Gamma(e)$ and

$$\mathrm{diag}\Gamma(g^p)=(1,1,\ldots) \quad . \qquad (3.26)$$

It follows that

$$\omega_J=\exp(2\pi i n_J/p), \qquad (3.27)$$

where n_J is selected from the set of integers $1,\ldots,p$, i.e.,

the eigenvalues ω_J of Γ are selected from among the p^{th} roots of unity. It may be that in a given representation $\Gamma(g)^t=\Gamma(e)$, where t divides p, but the argument does not depend on this.

In using (3.5), (3.6) we must determine which ω_J appear, and the multiplicity of appearance. Let us call δ_J the multiplicity (frequencu of appearance of a particular ω_J in (3.5)). Then (3.6) can be rewritten

$$\prod_{J=1}^{p}(1-z\omega_J)^{-\delta_J} \quad , \tag{3.28}$$

where $\sum_{J=1}^{p}\delta_J=1$, the dimension of Γ.

Consider the subgroup A, generated by g, consisting of all powers of g: $g,g^2,\ldots,g^p=e$. The irreducible represntations of A are lebeled by the p^{th} roots of unity:

$$g\rightarrow\gamma_J(g)=\exp(2\pi i n_J/p), \quad J=1,\ldots,p \quad . \tag{3.29}$$

A little consideration then shows that if we consider Γ of G as a representation of A (i.e., we subduce),

$$\Gamma \text{ of } G\downarrow\gamma_J \text{ of } A \ , \tag{3.30}$$

then

$$\delta_J=|A|^{-1}\sum_m\gamma_J(g^m)^*\chi(g^m) \ . \tag{3.31}$$

That is, the multiplicity δ_J is the reduction coefficient of Γ of G, upon γ_J of A. To find the δ_J one simply reads of the characters $\chi(g^m)$ of the cyclic subgroup and carries out the reduction (3.31) in the usual manner; prior to this one has constructed all the needed basic set of characters γ_J of A, as p^{th} roots of unity. In (3.31) $|A|=p$.

Assembling this we have

$$M(\Gamma,G;z)=|G|^{-1}\sum_g\prod_{J=1}^{p}\{1-z\gamma_J(g)\}^{-\delta_J} \quad . \tag{3.32}$$

Using the periodicity of the characters for finite groups, mentioned above, we have also verified that Eq. 3.32 follows from Eq. 3.21.

The merit of these two algorithms is that they facilitate the calculation of the Molien function by only using characters, which are generally more readily available than representations.

Before we apply these algorithms to the case where the group G is a space group we shall assemble some formulas for the elements of a crystal space group which will be used later.

Let the translation group T of the crystal be generated by the fundamental translation $\underline{a}_i$, i=1,2,3. Using periodic boundary conditions, we have

$$(e|\underline{a}_i)^{N_i}=(e|\underline{0}),\ i=1,2,3 \quad . \tag{3.33}$$

Then $|T| =N_1N_2N_3$. The set of all lattice translations

$$(e|\underline{R}_L)=(e|l_i\underline{a}_i) \quad , \tag{3.34}$$

$$-N_i/2\leq l_i<N_i/2 \quad , \ l_i \text{ integer, } i=1,2,3, \tag{3.35}$$

forms T. Sometimes below we denote a lattice vector by $\underline{R}$. It is simpliest to consider a cubic system with $N_1=N_2=N_3$; there is no loss of generality.

Call the space group G. The factor group G/T is isomorphic to a crystal point group P. Coset representatives in the decomposition of G with respect to T are

$$(\phi|\underline{\tau}) \text{ with } \begin{cases} \underline{\tau}=\underline{0} \\ \text{or} \\ \underline{\tau}=\text{a fractional translation.} \end{cases} \tag{3.36}$$

A general element g of G is

$$g=(\phi|\underline{t}) \ , \ \underline{t}=\underline{\tau}+\underline{R}_L \quad . \tag{3.37}$$

If required we may affix an index to ϕ and $\underline{\tau}$ such as ϕ_σ , $\underline{\tau}_\sigma$; other symbols will be defined as needed. Assume the rotational element ϕ has period p, so $\phi^p=e$. Then

$$g^p=(\phi|\underline{t})^p=(e|\underline{R}_p) \ , \tag{3.38}$$

where

$$\underline{R}_p=(\underline{t}+\phi\underline{t}+\ldots+\phi^{p-1}\underline{t})\equiv\{\phi\}^p\cdot\underline{t} \tag{3.39}$$

and

$$\{\phi\}^p\equiv\sum_{\lambda=0}^{p-1}(\phi)^\lambda \quad . \tag{3.40}$$

Thus

$$\underline{R}_p=p_i\underline{a}_i \qquad (p_i \text{ integer}) \tag{3.41}$$

is some lattice vector. The period of $\underline{R}_p$ will be N/q, $q\geq 1$ with q an integer. We find it simpler, and no less general, to choose q=1 so that the period of an element g depends on the period of its rotational part in a simple fashion:

$$g^{pN}=(e|\underline{0}) \quad . \tag{3.42}$$

We will need the element g^m. Take for g the expression 3.37. Then

$$g^m=(\phi^m|\{\phi\}^m\underline{t}) \quad . \tag{3.43}$$

In order to take advantage of the period of ϕ, we write for m:

$$m=\mu+lp \text{ with } \mu=1,\ldots,p;\ l=0,\ldots,N-1 \quad . \tag{3.44}$$

Then

$$\phi^m=\phi^\mu \tag{3.45}$$

and

$$\{\phi\}^m\underline{t}=\{\phi\}^{lp}\underline{t}+\{\phi\}^\mu\underline{t}=l\underline{R}_p+\{\phi\}^\mu\underline{t}=$$

$$=l\underline{R}_p+\{\phi\}^\mu\underline{t}-\underline{\tau}_\mu+\underline{\tau}_\mu=l\underline{R}_p+\underline{R}_\mu+\underline{\tau}_\mu \quad , \tag{3.46}$$

where

$$\underline{R}_\mu \equiv \{\phi\}^\mu \underline{t} - \underline{I}_\mu \tag{3.47}$$

is some lattice vector, and $\underline{I}_\mu$ is the fravtional (or zero) in the coset representative whose rotational part is ϕ^μ. Then

$$g^m = g^{\mu+1p} = (e|1\underline{R}_p)(e|\underline{R}_\mu)(\phi^\mu|\underline{I}_\mu) \ . \tag{3.48}$$

The element $g_\sigma^{-1} g^m g_\sigma$ will also be needed later. The element g is as before, in 3.37, while

$$g_\sigma \equiv (\phi_\sigma|\underline{I}_\sigma) \ . \tag{3.49}$$

Hence

$$g_\sigma^{-1} g^m g_\sigma = (e|\phi_\sigma^{-1}(\underline{R}_\mu + 1\underline{R}_p))((\phi^{\tilde{\mu}})^\sigma|\underline{t}_{\sigma\mu\sigma}) \tag{3.50}$$

where

$$(\phi^{\tilde{\mu}})^\sigma \equiv \phi_\sigma^{-1}\phi^\mu\phi_\sigma \tag{3.51}$$

and

$$\underline{t}_{\sigma\mu\sigma} \equiv (\phi_\sigma^{-1}\phi^\mu\underline{I}_\sigma + \phi_\sigma^{-1}\underline{I}_\mu - \phi_\sigma^{-1}\underline{I}_\sigma) \ . \tag{3.52}$$

The translation $\underline{t}_{\sigma\mu\sigma}$ is in general a sum of fractional plus lattice translation, and might be written

$$\underline{t}_{\sigma\mu\sigma} = \phi_\sigma^{-1}\underline{R}_{\mu\sigma} + \underline{I}_{\mu\sigma} \tag{3.53}$$

where $\underline{I}_{\mu\sigma}$ is the fractional associated with rotational part $(\phi^{\tilde{\mu}})^\sigma$ in the coset representative, while $\underline{R}_{\mu\sigma}$ is defined by (3.53) and is a lattice vector.

We shall be concerned with the Molien function for irreducible representation Γ of space group G. The construction of Γ of G and of χ is well known,[36] and we shall simply cite some relevant expressions.

Let the irreducible representation Γ of the space group G be labeled $*\underline{k}n$ where $*\underline{k} = (\underline{k}_1 = \underline{k}, \underline{k}_2, \ldots, \underline{k}_\sigma = \phi_\sigma\underline{k}, \ldots, \underline{k}_s)$ and n refers to the allowable little group irreducible representation of $G(\underline{k})$. The canonical wave vector is $\underline{k}$, and $G(\underline{k})$

is the space group of the wave vector $\underline{k}$. Coset representatives in the canonical decomposition of G with respect to $G(\underline{k})$ are g_σ:

$$G=G(\underline{k})+g_2G(\underline{k})+\ldots+g_\sigma G(\underline{k})+\ldots+g_s G(\underline{k}) \quad . \tag{3.54}$$

We always reserve the index σ for such representatives. Then

$$\chi^{*\underline{k}n}(g)=\sum_{\sigma=1}^{s} \chi^{\cdot(\underline{k})(n)}(g_\sigma^{-1}gg_\sigma) \tag{3.55}$$

and $\chi^{\cdot(\underline{k})(n)}(h)=0$ if $h\notin G(\underline{k})$. Later we require the character of g^m.

Consider the Abelian subgroup A generated by group element g. Because we take the period of the elments in the space group to be pN the group A has pN distinct irreducible representations given by

$$g\rightarrow\gamma_J(g)=\exp(2\pi i n_J/pN) \quad , \quad n_J=1,\ldots,pN \quad ,$$
$$J=1,\ldots,pN \quad . \tag{3.56}$$

Below it will prove convinient to take $n_J=J$ and

$$n_J=J=j+\nu N, \quad j=1,\ldots,N; \quad \nu=0,\ldots,p-1 \quad . \tag{3.57}$$

Of course, we still retain the same number of roots this way, but mearly achieve a simpler labeling. Equivalently, j is an integer (mod N), and ν is an integer (mod p).

Recalling Eqs. 3.26-3.32, we se that the $\gamma_J(g)$ are the possible eigenvalues ω_J which occur in the expression for the Molien function.

We are now in position to assemble all the previous results to calculate the Molien function for representation Γ (labeled $*\underline{k}n$) of G. Our strategy must be to compute the subduction coefficients δ_J and the corresponding eigenvalues γ_J. Ther is no difficulty in principle since we are merely evalu-

ating the sum 3.31:

$$\delta_J = |A|^{-1} \sum_m \gamma_J(g^m)^* \chi(g^m) \quad . \tag{3.58}$$

The sum goes over all elements inthe cyclic subgroup A generated by g. However, because Γ is an induced representation and the structure of χ reflects this as in Eq. 3.55, the calculation is formaly rather untidy. Her we shall simplify the formulas as much as seems possible at present.

We requiere that

$$\begin{aligned}
\chi^{*\underline{k}n}(g^m) &= \sum_{\sigma=1}^{s} \dot{\chi}^{(\underline{k})(n)}(g_\sigma^{-1} g^m g_\sigma) = \\
&= \sum_{\sigma=1}^{s} \dot{\chi}^{(\underline{k})(n)}((e|\phi_\sigma^{-1}\cdot(l\underline{R}_p + \underline{R}_\mu))((\phi^{\tilde{\mu}})^\sigma|\underline{t}_{\sigma\mu\sigma})) = \\
&= \sum_\sigma \exp\{-i\underline{k}_\sigma\cdot(l\underline{R}_p + \underline{R}_\mu)\}\dot{\chi}^{(\underline{k})(n)}((\phi^{\tilde{\mu}})^\sigma|\underline{t}_{\sigma\mu\sigma}) = \\
&= \sum_\sigma \exp\{-i(l\underline{k}_\sigma\cdot\underline{R}_p + \underline{k}_\sigma\cdot\underline{R}_\mu + \underline{k}_\sigma\cdot\underline{R}_{\mu\sigma})\}\times \\
&\quad \times \dot{\chi}^{(\underline{k})(n)}((\phi^{\tilde{\mu}})^\sigma|\underline{\tau}_{\mu\sigma}) \quad ,
\end{aligned} \tag{3.59}$$

where $\underline{k}_\sigma = \phi_\sigma \underline{k}$ is one of the members of $^*\underline{k}$, not equivalent to $\underline{k}$, since $(\phi_\sigma|\underline{\tau}_\sigma)$ is not in $G(\underline{k})$. Note that in 3.59 the label l hs been separated out,and we have taken $m = \mu + pl$ (see 3.44) and used Eqs. 3.50-3.53.

Then, returning to 3.58 and replacing the sum on m by appropriate sums on μ and l, we have as an intermediate step

$$\delta_J = \sum_{\sigma=1}^{s} p^{-1} \sum_{\mu=1}^{p} N^{-1} \sum_{l=0}^{N-1} \gamma_J(g^{\mu+lp})^* \dot{\chi}^{(\underline{k})(n)}(g_\sigma^{-1} g^{\mu+lp} g_\sigma) \quad . \tag{3.60}$$

Now write, following 3.56 and 3.59, $m = \mu + pl$, and $n_J = j + \nu N$, so that

$$\begin{aligned}
\gamma_J(g^m)^* &= \exp\{-2\pi i(\mu+pl)(j+\nu N)/pN\} = \\
&= \exp\{-2\pi i(\mu j/pN + \mu\nu/p + lj/N)\} \quad .
\end{aligned} \tag{3.61}$$

It is already clear here that some indices are redundant, and

we shall eliminate j shortly.

The first step is now to calculate the sum on l, and we isolate the relevant terms in 3.60 to obtain

$$N^{-1}\sum_{l=0}^{N-1}\exp\{-il(2\pi j/N+\underline{k}_\sigma\cdot\underline{R}_p)\}=\Delta(j/N+\underline{k}_\sigma\cdot\underline{R}_p/2\pi). \quad (3.62)$$

This will immediately be recognized as a "lattice delta"

$$\Delta(y)=\begin{cases}1 \text{ if } y=\text{integer},\\ 0 \text{ otherwise.}\end{cases} \quad (3.63)$$

Taking account of the restrictions on j (an integer mod N) and $\underline{k}_\sigma\cdot\underline{R}_p=2\pi(\text{integer})/N$, we find

$$2\pi j/N+\underline{k}_\sigma\cdot\underline{R}_p=0 \quad (3.64)$$

as the only permitted value of j, which now allows us to write

$$\delta_J=\sum_{\sigma=1}^{s}\delta_{\nu\sigma}\Delta(j/N+\underline{k}_\sigma\cdot\underline{R}_p/2\pi)\ , \quad (3.65)$$

where we define

$$\delta_{\nu\sigma}\equiv p^{-1}\sum_{\mu=1}^{p}\exp\{-i(2\pi\mu\nu/p+\underline{k}_\sigma\cdot(\underline{R}_\mu+\underline{R}_{\mu\sigma}-\mu\underline{R}_p/p))\}\times$$
$$\times\dot{\chi}^{(\underline{k})(n)}((\phi^{\tilde{\mu}})^\sigma|_{\underline{\tau}_{\mu\sigma}})\ . \quad (3.66)$$

($\delta_{\nu\sigma}$ should not be confused with a Kronecker delta $\delta_{\nu,\sigma}$ which we denote with comma between indices). An interesting note about 3.66 is that there is no dependence on N.

Although it may appear chumbersome, Eqs. 3.65, 3.66 may be readily used in computations. It is assumed that the space group irreducible representations are known, so that, for each $*\underline{k}n$, the set of coset representatives in $G(\underline{k})$ is known, as are the dotted charecters $\dot{\chi}^{(\underline{k})(n)}$, and the set of elements g_σ. Computation of the translations $\underline{R}_p$, $\underline{R}_\mu$, $\underline{R}_{\mu\sigma}$ is straightforward and so is the evaluation of the sum 3.66.

In the same fashion that the calculation of δ_J simplifies, so does the calculation of each term in 3.32, which is

$$\prod_J \{1-z\gamma_J(g)\}^{-\delta_J} \quad , \tag{3.67}$$

and, substituting $J=j+\nu N$ as before, we find this becomes

$$\prod_{\nu=0}^{p-1} \prod_{j=1}^{N} \{1-z\exp(2\pi i(j+\nu N)/pN)\}^{-\delta_{j+\nu N}} \quad . \tag{3.68}$$

Now we may use Eq. 3.65 and eliminate index j in favor of σ as in 3.64, and thus we change the range of the product appropriately, so that 3.68 becomes

$$\prod_{\nu=0}^{p-1} \prod_{\sigma=1}^{s} \{1-z\exp(i(2\pi\nu-\underline{k}_\sigma\cdot\underline{R}_p)/p)\}^{-\delta_{\nu\sigma}} \quad . \tag{3.69}$$

In order to exhibit these formulas in more compact form, let us define the quantities

$$\omega_p \equiv \exp(2\pi i/p) \quad , \tag{3.70}$$

$$\gamma_{\sigma\mu} \equiv \exp\{-i\underline{k}_\sigma\cdot(\underline{R}_\mu+\underline{R}_{\mu\sigma})/p\} \quad . \tag{3.71}$$

Of course these allrefer to a single space group element g. Then

$$\delta_{\nu\sigma}=p^{-1}\sum_{\mu=1}^{p}(\omega_p^*)^{\mu\nu}(\gamma_{\sigma p}^*)^{\mu}(\gamma_{\sigma\mu})^{p}\chi(\underline{k})(n)((\phi^{\tilde{\mu}})^{\sigma}|\underline{\tau}_{\mu\sigma}) \tag{3.72}$$

and

$$M(*\underline{k}n,G;z)=|G|^{-1}\sum_{g}\prod_{\nu=0}^{p-1}\prod_{\sigma=1}^{s}\{1-z\gamma_{\sigma p}(\omega_p)^{\nu}\}^{-\delta_{\nu\sigma}}. \tag{3.73}$$

We continue with Eq. 3.73 and reduce it to a form in which it appears as asum of partial Molien functions, each lebeled by an index derived from an index of class of the point group P of space group G.

Let P=G/T. We call the k^{th} conjugacy class of P $C_k(P)$, with elements

$$C_k(P):\phi_{ki} \ , \ i=1,\ldots,c_k \quad , \tag{3.74}$$

where ϕ_{ki} is a rotation-reflection.

Call the k th conjugacy class of G $C_{k\alpha}(G)$, with elements

$$t_{k\alpha i} \ (e|\underline{R}_{k\alpha i})(\phi_{ki}|\underline{\tau}_{ki}) \quad , \ i=1,\ldots,c_k \quad . \tag{3.75}$$

The index α willrefer to those lattice translations associated with ϕ_{ki}, and $\underline{\tau}_{ki}$ is the canonical fractional; $t_{k\alpha i}$ is an element in T. To understand the structure of the conjugacy classes of G, form the conjugate of 3.75 with respect to general element $g=(\phi|\underline{t})$, where $\underline{t}=\underline{\tau}+\underline{R}$ with $\underline{\tau}$ the canonical fractional for ϕ and $\underline{R}$ a lattice vector as in Eq.3.27. Then

$$g^{-1}t_{k\alpha i}g_{ki}g=t'_{k\alpha j}g_{kj} \tag{3.76}$$

with

$$g_{kj}=(\phi^{-1}\phi_{ki}\phi|\underline{\tau}_{kj})\equiv(\phi_{kj}|\underline{\tau}_{kj}) \quad , \tag{3.77}$$

$$t'_{k\alpha j}\equiv(e|\phi^{-1}(\underline{R}_{k\alpha i}+\underline{R}')) \ , \tag{3.78}$$

and

$$\phi^{-1}\underline{R}'\equiv(\phi_{kj}-e)\phi^{-1}\underline{t}+\phi^{-1}\underline{\tau}_{ki}-\underline{\tau}_{kj} \quad . \tag{3.79}$$

When g runs through all elements in G, one will obtain on the right side of 3.76 the set of coset representatives g_{ki}, i=1, ...,c_k whose rotational parts are all the members of the conjugacy class $C_k(P)$ of Eq. 3.74. Each such fixed rotational part (fixed k and i) will be associated with a set of translations, e.g., $t_{k\alpha i}$ which is a subset of T. For example if ϕ commutes with ϕ_{ki}, then the set 3.78 will occur with

$$\phi^{-1}\underline{R}'=(\phi_{ki}-e)\phi^{-1}\underline{t}+\phi^{-1}\underline{\tau}_{ki}-\underline{\tau}_{ki} \quad . \tag{3.80}$$

To label a class in G, we require an index k referring to set ϕ_{ki} and an index α reffering to the particular subset

of translations accompanying a specified representative such as g_{ki}. For fixed ki a subset $T_{k\alpha i}$ of translatioms occurs in class $C_{k\alpha}(G)$ accompanying g_{ki}. Then for fixed ki, the decomposition of T with respect to the class lebel α is disjoint.

$$T=\sum_{\alpha} T_{k\alpha i} \quad , \quad T_{k\alpha i} \equiv \{t_{k\alpha i}\} \quad . \tag{3.81}$$

Thus a single class $C_k(P)$ in P, with c_k elements gives rise to several classes $C_{k\alpha}(G)$ in G.

Let f(t) be a function of the translations t of T. Then for fixed ki

$$\sum_{t\in T} f(t)=\sum_{\alpha} \sum_{t\in T_{k\alpha i}} f(t) \quad , \text{ fixed ki} \quad . \tag{3.82}$$

Let χ be a character in a representation of G; then

$$\chi(t_{k\alpha i}g_{ki})=\chi(t_{k\alpha j}g_{kj}) \quad . \tag{3.83}$$

Since χ is a class function, it is independent of i, j since these refer to the same class.

Now let $F(\chi)$ be a function on the characters of Γ of G, and let t be an arbitrary translation in T. Then

$$\sum_{t\in T} F(\chi(tg_{ki}))=\sum_{\alpha}\sum_{t\in T_{k\alpha i}} F(\chi(tg_{ki}))=F_k \quad . \tag{3.84}$$

The last step follows from 3.82 and 3.83, and now 3.84 can be used to rewrite the expression for the Molien function.

Returning to the expression 3.7 for Molien function, we may write, for g an element of the space group G,

$$M(\Gamma,G;z)=|G|^{-1}\sum_{g} m(\Gamma,g;z) \quad . \tag{3.85}$$

Letting $g\equiv tg_{ki}$

$$\begin{aligned} M(\Gamma,G;z) &= |P|^{-1}\sum_{k}\sum_{i}|T|^{-1}\sum_{t} m(\Gamma,tg_{ki};z)= \\ &= |P|^{-1}\sum_{k} c_k \bar{m}(\Gamma,g_k;z), \end{aligned} \tag{3.86}$$

where

$$\bar{m}(\Gamma,g_k;z)\equiv|T|^{-1}\sum_t m(\Gamma,tg_k;z) \quad . \tag{3.87}$$

The last step in 3.86 follows owing to the use of 3.84. The symbol g_k is a typical element or coset representative corresponding to class $C_k(P)$. Then, instead of Eq. 3.73, we write

$$\bar{m}(\Gamma,g_k;z)=|T|^{-1}\sum_t \prod_{\nu=1}^{p}\prod_{\sigma=1}^{s}\{1-z\gamma_{\sigma p}(\omega_p)^{\nu}\}^{-\delta_{\nu\sigma}} . \tag{3.88}$$

All quantities refer to elements tg_k in G.

At the end of this chapter we verify dimensionality formula give below Eq.3.28, which shows that the degree of the polynomial in the denominator is equal to the dimensionality of the representation Γ. To verify this property in Eq. 3.73 we have to show that

$$\sum_{\sigma=1}^{s}\sum_{\nu=0}^{p-1}\delta_{\nu\sigma}=sl_n \quad , \tag{3.90}$$

where sl_n is the dimensionality of the irreducible representation $*\underline{k}n$ of G and l_n is the dimensionality of the irreducible representation $D^{(\underline{k})(n)}$ of $G(\underline{k})$. Since ν appears in 3.72 only in $(\omega_p^*)^{\mu\nu}$, the sum over ν will give

$$p^{-1}\sum_{\nu=0}^{p-1}(\omega_p^*)^{\mu\nu}=\Delta(\mu/p)=\delta_{\mu,p} \quad , \tag{3.91}$$

where we took into account the fact that μ is restricted to the values $1,\ldots,p$. Thus by 3.91 we may eliminate the summation over μ, leaving only terms $\mu=p$. Then from the definition of $\gamma_{\sigma\mu}$ we see that $(\gamma_{\sigma p}^*)^{\mu}(\gamma_{\sigma\mu})^{p}\big|_{\mu=p}=1$, so that the left-hand side of 3.90 reduces to:

$$\sum_{\sigma=1}^{s} \sum_{\sigma=1}^{p} \delta_{\nu\sigma} = \sum_{\sigma=1}^{s} \dot{\chi}^{(\underline{k})(n)}((\tilde{\phi}^{p})^{\sigma}|\underline{\tau}_{p\sigma}) \quad . \tag{3.92}$$

However, $(\tilde{\phi}^{p})^{\sigma}=e$, by 3.52, and thus $\underline{\tau}_{p\sigma}=\underline{0}$. Finally since $\dot{\chi}^{(\underline{k})(n)}(e|\underline{0})=1_n$ (independent of σ), 3.92 reduces to 3.90.

The formulae obtained here will be used in the following chapter in which we will calculate the Molien functions, and subsequently quartic invariants, for irreducible representations of space group O_h^3-Pm3n.

CHAPTER 4

Molien Generating Function and Invariant Polynomials for Space Group O_h^3 [30,37]

In Chapter 2 we have used Landau Theory to analyze second order structural phase transitions in A-15 systems having symmetry O_h^3. Since in Chapter 6 we will apply a renormalization-group technique to these systems, we will need to calculate quartic invariants for some irreducible representations of space group O_h^3. Therefore we will calculate the Molien functions and all quartic invariants for representations *$\underline{R}$n and *$\underline{X}$n. Before dealing with these representations we shall discuss, as an illustration, the representations *$\underline{\Gamma}$n.

Since O_h^3 is nonsymmorphic, the calculation of the Molien function in this case may illustrate some typical problems which arise in such calculations for space groups. The results are also of interest since they may reval new features peculiar to space groups.

The irreducible representations of this space group

have been given by Gorzkowski[22] and in addition are listed in the standard compilation Miller and Love.[28] We follow these authors' notations and we shall also indicate connection to another notation used by Gor'kov[9] (see Table 4.1).

Representations *$\underline{\Gamma}$n

At the center of the Brillouin zone, the group $G(\underline{\Gamma})$ is the entire space group and the factor group $G(\underline{\Gamma})/T$ is a group isomorphic to point group O_h since all translations in T map into the identity. All irreducible representations of O_h are well known as are the irreducible character system.

In Table 4.1 we give: class multiplicity, coset representatives in $G(\underline{\Gamma})/T \sim O_h$ (first column), then in succeeding columns for each irreducible representation *$\underline{\Gamma}$n the partial Molien function which arises by summing over all elements in T. The weighted sum of all the partial Molien functions as in Eq. 3.86 gives $M(*\underline{\Gamma}n, O_h^3; z)$, and these are listed in Table 4.3 where the first seven rows refer to *$\underline{\Gamma}$n. The notation of Miller and Love[28] is used. The result for the fundamental representation *$\underline{\Gamma}$4- of O_h^3 agrees with a result of Meyer,[38] who gave Molien functions for the fundamental representations of all point groups.

Representations *$\underline{X}$n

At the point $\underline{X}=(0,0,\pi/a)$ in the Brillouin zone the allowable irreducible representations of $G(\underline{X})$ may be considered as ray representations of $G(\underline{X})/T \sim D_{4h}$ with nontrivial factor systems.[39] All allowable $(\underline{X})(n)$, n=1,2,3,4, are two dimensional, and the *$\underline{X}$n are six dimensional. Some of these

TABLE 4.1

Partial Molien Function $\bar{m}(\Gamma,g_k;z)$ (text (3.86)) for Irreducible Representation $*\underline{\Gamma}n$ of O_h^3 .[a] In the Tables: $P_n=1-z^n$; $Q_n=1+z^n$; $R_4(n)=1+nz^2+z^4$; $S_2=1-z+z^2$; $T_2=1+z+z^2$.

	$*\underline{k}n$	$*\underline{\Gamma}1+$	$*\underline{\Gamma}1-$	$*\underline{\Gamma}2+$	$*\underline{\Gamma}2-$	$*\underline{\Gamma}3+$	$*\underline{\Gamma}3-$	$*\underline{\Gamma}4+$	$*\underline{\Gamma}4-$	$*\underline{\Gamma}5+$	$*\underline{\Gamma}5-$
c_k	g_k	$\bar{m}(*\underline{k}n,g_k;z)$									
1	$(e\|\underline{0})$	$1/P_1$	$1/P_1$	$1/P_1$	$1/P_1$	$1/P_1^2$	$1/P_1^2$	$1/P_1^3$	$1/P_1^3$	$1/P_1^3$	$1/P_1^3$
8	$(c_3\|\underline{0})$	$1/P_1$	$1/P_1$	$1/P_1$	$1/P_1$	$1/T_2$	$1/T_2$	$1/P_3$	$1/P_3$	$1/P_3$	$1/P_3$
3	$(c_4^2\|\underline{0})$	$1/P_1$	$1/P_1$	$1/P_1$	$1/P_1$	$1/P_1^2$	$1/P_1^2$	$1/P_2Q_1$	$1/P_2Q_1$	$1/P_2Q_1$	$1/P_2Q_1$
1	$(i\|\underline{0})$	$1/P_1$	$1/Q_1$	$1/P_1$	$1/Q_1$	$1/P_1^2$	$1/Q_1^2$	$1/P_1^3$	$1/Q_1^3$	$1/P_1^3$	$1/Q_1^3$
8	$(s_6\|\underline{0})$	$1/P_1$	$1/Q_1$	$1/P_1$	$1/Q_1$	$1/T_2$	$1/S_2$	$1/P_3$	$1/Q_3$	$1/P_3$	$1/Q_3$
3	$(\sigma\|\underline{0})$	$1/P_1$	$1/Q_1$	$1/P_1$	$1/Q_1$	$1/P_1^2$	$1/Q_1^2$	$1/P_2Q_1$	$1/P_1P_2$	$1/P_2Q_1$	$1/P_1P_2$
6	$(c_2\|\underline{\tau})$	$1/P_1$	$1/P_1$	$1/Q_1$	$1/Q_1$	$1/P_2$	$1/P_2$	$1/P_1P_2$	$1/P_1P_2$	$1/P_2Q_1$	$1/P_2Q_1$
6	$(c_4\|\underline{\tau})$	$1/P_1$	$1/P_1$	$1/Q_1$	$1/Q_1$	$1/P_2$	$1/P_2$	$1/Q_1Q_2$	$1/Q_1Q_2$	$1/P_1Q_2$	$1/P_1Q_2$
6	$(\sigma_v\|\underline{\tau})$	$1/P_1$	$1/Q_1$	$1/Q_1$	$1/P_1$	$1/P_2$	$1/P_2$	$1/P_1P_2$	$1/P_2Q_1$	$1/P_2Q_1$	$1/P_1P_2$
6	$(s_4\|\underline{\tau})$	$1/P_1$	$1/Q_1$	$1/Q_1$	$1/P_1$	$1/P_2$	$1/P_2$	$1/Q_1Q_2$	$1/P_1Q_2$	$1/P_1Q_2$	$1/Q_1Q_2$

[a] Notation follows Ref.28.

representations have been used in recent theories of properties of these systems.[9]

In Table 4.2 we give the functions $\bar{m}(*\underline{X}n, g_k; z)$ for n= 1,2,3,4. In Table 4.3, lines 8 and 9, the full Molien function $M(*\underline{X}n, O_h^3; z)$ is given, and as we note representations *X1 and *X2 have same Molien functions. However, it does not follow that two representations with identical Molien functions have identical invariants (up to a similarity transformation).

In the case of these representations, however, as can be seen from Tables 4.4 and 4.5 matrix groups *X1 and *X2 as well as *X3 and *X4 are identical and thus respective invariants are identical too.

Representations *Rn

At the point $\underline{R}=(\pi/a,\pi/a,\pi/a)$ in the Brillouin zone allowable irreducible representations of $G(\underline{R})$ are ray representations of $G(\underline{R})/T=O_h$. The factor system is nontrivial.[39] Allowable irreducible representations *Rn are two dimensional (n=1,2,3) and six dimensional (n=4). The six dimensional *R4 is unusual: it was used in a recent theory of the electronic properties of the A-15 systems.[11] Representations *R2 and *R3 are time reverse, and it proves interesting to consider the four dimensional physically irreducible representation *R2⊕*R3.

In Table 4.2, last four columns, we list the $\bar{m}(*\underline{R}n, g_k; z)$. In Table 4.3, last four rows, we give the Molien functions $M(*\underline{R}n, O_h^3; z)$, including for a physically irreducible *R2⊕*R3. We see from Table 4.3 that representation *R4 has identical Molien function as representations *X3 and *X4. In

TABLE 4.2

Partial Molien Function $\bar{m}(\Gamma,g_k;z)$ for Irreducible Representations *$\underline{X}$n, and *$\underline{R}$n of O_h^3.[a] See Table 4.1 heading.

	*$\underline{k}$n	*$\underline{X}$1,2	*$\underline{X}$3,4	*$\underline{R}$1	*$\underline{R}$2,3	*$\underline{R}$2•*$\underline{R}$3	*$\underline{R}$4
c_k	g_k	$\bar{m}(*\underline{k}n,g_k;z)$					
1	$(e\|\underline{0})$	Q_2^3/P_2^6	Q_2^3/P_2^6	Q_2/P_2^2	Q_2/P_2^2	$R_4(6)/P_2^4$	$Q_2R_4(14)/P_2^6$
8	$(c_3\|\underline{0})$	Q_6/P_6^2	Q_6^2/P_6	Q_2/P_2^2	P_4/P_6	$R_4(3)/R_4(1)^2$	Q_6/P_6^2
3	$(c_4^2\|\underline{0})$	Q_2/P_2^4	Q_2^3/P_2^6	Q_2/P_2^2	Q_2/P_2^2	$R_4(6)/P_2^4$	Q_2/P_2^4
1	$(i\|\underline{0})$	$1/P_2^3$	$1/P_2^3$	$1/P_2$	$1/P_2$	$1/P_2^2$	$1/P_2^3$
8	$(s_6\|\underline{0})$	$1/P_6$	$1/P_6$	$1/P_2$	P_2^2/P_6	P_2/P_6	$1/P_6$
3	$(\sigma\|\underline{0})$	Q_2^2/P_2^5	$1/P_2^3$	$1/P_2$	$1/P_2$	$1/P_2^2$	$1/P_2^3$
6	$(c_2\|\underline{\tau})$	$Q_4/P_2P_4^2$	$Q_4/P_2P_4^2$	$1/P_2$	$1/P_2$	$1/P_2^2$	$1/P_2^3$
6	$(c_4\|\underline{\tau})$	$1/P_4Q_2$	$Q_4/P_2P_4^2$	$1/P_2$	$1/P_2$	$1/P_2^2$	$1/P_2Q_2^2$
6	$(\sigma_v\|\underline{\tau})$	$Q_4/P_4^2Q_2$	$Q_4/P_4^2Q_2$	$1/Q_2$	$1/Q_2$	$1/Q_2^2$	$1/Q_2^3$
6	$(s_4\|\underline{\tau})$	$1/P_2P_4$	$Q_4/P_4^2Q_2$	$1/Q_2$	$1/Q_2$	$1/Q_2^2$	$1/P_2^2Q_2$

[a] Notation follows Ref.28. Representations *$\underline{X}$1,*$\underline{X}$2,*$\underline{X}$3,*$\underline{X}$4 are called $*X_2$, $*X_4$, $*X_1$, $*X_3$, respectively, in Ref.9.

TABLE 4.3

Molien Generating Function $M(\Gamma,G;z)$ for Irreducible Representations $*\underline{\Gamma}n$, $*\underline{X}n$, $*\underline{R}n$ of O_h^3 .

Irrep. $*\underline{k}n$	$M(*\underline{k}n, O_h^3; z)$
$*\underline{\Gamma}1+$	$\frac{1}{(1-z)}$
$*\underline{\Gamma}1-$, $*\underline{\Gamma}2\pm$	$\frac{1}{(1-z^2)}$
$*\underline{\Gamma}3+$	$\frac{1}{(1-z^2)(1-z^3)}$
$*\underline{\Gamma}3-$	$\frac{1}{(1-z^2)(1-z^6)}$
$*\underline{\Gamma}4+$	$\frac{1}{(1-z^2)(1-z^3)(1-z^4)}$
$*\underline{\Gamma}4-$, $*\underline{\Gamma}5-$	$\frac{1}{(1-z^2)(1-z^4)(1-z^6)}$
$*\underline{\Gamma}5+$	$\frac{1+z^9}{(1-z^2)(1-z^4)(1-z^6)}$
$*\underline{X}1,2$	$\frac{1+z^4+3z^6+5z^8+z^{10}+z^{12}}{(1-z^2)(1-z^4)^3(1-z^6)^2}$
$*\underline{X}3,4$, $*\underline{R}4$	$\frac{1+2z^4+5z^6+11z^8+9z^{10}+11z^{12}+6z^{14}+3z^{16}}{(1-z^2)(1-z^4)^3(1-z^6)^2}$
$*\underline{R}1$	$\frac{1}{(1-z^2)(1-z^4)}$
$*\underline{R}2,3$	$\frac{1}{(1-z^4)(1-z^6)}$
$*\underline{R}2 \blacklozenge *\underline{R}3$	$\frac{1+z^2+2z^4+4z^6+8z^8+4z^{10}+2z^{12}+z^{14}+z^{16}}{(1-z^4)^2(1-z^6)^2}$

effect, it is possible to find a similarity transformation which would transform a matrix group *R4 into a group *X3 (identical to *X4). Also, matrix groups *R2 and *R3 are identical and thus their Molien functions as well as invariants are identical.

In order to construct invariants explicitely we will use a projection operator P_1 defined for arbitrary group G as:

$$P_1 \equiv |G|^{-1} \sum_{g \in G} P_g \quad . \tag{4.1}$$

Where P_g is an operator acting on arbitrary function f(r) as:

$$\{P_g f\}(r) \equiv f(g^{-1} r) \quad . \tag{4.2}$$

Then, any function f generates a G-invariant function f_1 defined by:

$$f_1 \equiv P_1 f \quad . \tag{4.3}$$

In the specific case when f is a monomial of degree n in the basis functions ψ_i , i=1,...,l of an l-dimensional representation Γ of G, i.e., when

$$P_g \psi_i = \sum_j \Gamma(g)_{ji} \psi_j \quad , \quad i,j=1,\ldots,l; \ \forall g \in G, \tag{4.4}$$

and

$$f = \psi_{i_1} \psi_{i_2} \ldots \psi_{i_n} \quad , \tag{4.5}$$

function f_1 is given, with the aid of Eq. 4.1, by:

$$f_1 = |G|^{-1} \sum_g \sum_{j_1,\ldots,j_n} \Gamma(g)_{j_1 i_1} \ldots \Gamma(g)_{j_n i_n} \psi_{j_1} \ldots \psi_{j_n} \quad . \tag{4.6}$$

Also it is then obvious that a sum $|G|^{-1} \sum_g$ can be replaced by the sum $|\Gamma|^{-1} \sum_{\Gamma(g)}$.

Before we start calculating quartic invariants for representations *Xn and *Rn we would like to emphasize that although Molien function is independent of a similarity transformation on Γ, invariants are dependent upon the matrixform used for the irreducible representation. Thus, we will give in Tables 4.4 to 4.9 explicitely matrix groups *Xn and *Rn for which we calculate quartic invariants.

The matrix group of the representations *X1 and *X2 is given in Table 4.4. The basis functions of these representations are denoted $\psi_1,\bar{\psi}_1,\psi_2,\bar{\psi}_2,\psi_3,\bar{\psi}_3$. From Table 4.3 we see that for these representations there are five independent quartic invariants. These invariants we list in Table 4.10.

For the representations *X3 and *X4 matrix group is given in Table 4.5, and basis functions are $\psi_1,\bar{\psi}_1,\psi_2,\bar{\psi}_2,\psi_3,\bar{\psi}_3$. In this case, as can be seen from Table 4.3, there are six independent quartic invariants which we list in Table 4.10.

Irreducible representation *R1 is two dimensional, so we have basis functions ψ_1 and ψ_2. The matrix group for this representation is given in Table 4.6. From the corresponding Molien function (Table 4.3) it is clear that there are two independent quartic invariants which we give in Table 4.11.

Conjugate complex representations *R2 and *R3 form the identical matrix group given in Table 4.7, whose basis functions we take to be ψ_1 and ψ_2. There is only one quartic invariant which we give in Table 4.11. However, for physical applications we are interested in physically irreducible representation *R2⊕*R3 whose real matrix group we give in Table

TABLE 4.4

Matrix Group for Irreducible Representations *X1 and *X2 .

Matrix[a]	Number of different matrices
$\pm A_\pm$ 0 0 0 $\pm A_\pm$ 0 0 0 $\pm A_\pm$	$2^3 2^3 = 64$
0 0 $\pm A_\pm$ $\pm A_\pm$ 0 0 0 $\pm A_\pm$ 0	64
0 $\pm A_\pm$ 0 0 0 $\pm A_\pm$ $\pm A_\pm$ 0 0	64
0 0 $\pm B_\pm$ 0 $\pm B_\pm$ 0 $\pm B_\pm$ 0 0	64
$\pm B_\pm$ 0 0 0 0 $\pm B_\pm$ 0 $\pm B_\pm$ 0	64
0 $\pm B_\pm$ 0 $\pm B_\pm$ 0 0 0 0 $\pm B_\pm$	64
Order of the matrix group:	384

[a] All ± signs are independent; $A_+ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $A_- = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $B_+ = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $B_- = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$.

TABLE 4.5

Matrix Group for Irreducible Representations *X3 and *X4 .

Matrix[a)]	Number of different matrices
A_j 0 0 0 A_j 0 0 0 A_j	$2^3 2=16$
0 0 A_j A_j 0 0 0 A_j 0	16
0 A_j 0 0 0 A_j A_j 0 0	16
0 0 B_j 0 B_j 0 B_j 0 0	16
B_j 0 0 0 0 B_j 0 B_j 0	16
0 B_j 0 B_j 0 0 0 0 B_j	16
Order of the matrix group:	96

a) All ± signs are independent; j=1,2; $A_1=A_+$, $A_2=A_-$, $B_1=-iB_+$, $B_2=-iB_-$ (see Table 4.4).

TABLE 4.6

Matrix Group for Irreducible Representation *R1 .

Matrix[a]	Number of different matrices
$\pm\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	2
$\pm\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	2
$\pm\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	2
$\pm\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$	2
Order of the matrix group:	8

a) All ± signs are independent.

TABLE 4.7

Matrix Group for Irreducible Representations *R2 and *R3 .

Matrix[a]	Number of different matrices
$\begin{pmatrix}\pm1 & 0\\ 0 & \pm1\end{pmatrix}$	$2^2=4$
$\begin{pmatrix}\pm\lambda^2 & 0\\ 0 & \pm\lambda\end{pmatrix}$	4
$\begin{pmatrix}\pm\lambda & 0\\ 0 & \pm\lambda^2\end{pmatrix}$	4
$\begin{pmatrix}0 & \pm1\\ \pm1 & 0\end{pmatrix}$	4
$\begin{pmatrix}0 & \pm i\lambda^2\\ \pm i\lambda & 0\end{pmatrix}$	4
$\begin{pmatrix}0 & \pm i\lambda\\ \pm i\lambda^2 & 0\end{pmatrix}$	4
Order of the matrix group:	24

a) All ± signs are independent; $\lambda=e^{2\pi i/3}$.

TABLE 4

Matrix Group for the Representation *R2◆*R3.

Matrix[a]	Number of different matrices
$\pm\begin{pmatrix} A_j & 0 \\ 0 & A_j \end{pmatrix}$ $j=1,2,3,4$	$2\times4=8$
$\pm\frac{1}{2}\begin{pmatrix} A_j & \alpha A_k \\ -\alpha A_k & A_j \end{pmatrix}$ $\alpha=\pm\sqrt{3}$ $(j,k)=(1,2),(2,1),(3,4),(4,3).$	$2\times2\times4=16$
Order of the matrix group:	24

a) $A_1,A_2,A_3,A_4,0$ here is the same as $A_1,B_1,A_2,B_2,0$, respectively, of Table 4.5.

TABLE 4.9

Matrix Group for Irreducible Representation *R4.

Matrix[a]	Number of different matrices
$\begin{pmatrix} A & 0 \\ 0 & \pm A \end{pmatrix}$ $A=\begin{pmatrix}\pm1&0&0\\0&\pm1&0\\0&0&\pm1\end{pmatrix},\begin{pmatrix}0&0&1\\\pm1&0&0\\0&\pm1&0\end{pmatrix},\begin{pmatrix}0&1&0\\0&0&\pm1\\\pm1&0&0\end{pmatrix}.$	$2\times3\times2^3=48$
$\begin{pmatrix} 0 & B \\ \pm B & 0 \end{pmatrix}$ $B=\begin{pmatrix}0&0\pm1&0\\0\pm1&0&0\\\pm1&0&0\end{pmatrix},\begin{pmatrix}0\pm1&0&0\\\pm1&0&0\\0&0\pm1&0\end{pmatrix},\begin{pmatrix}\pm1&0&0\\0&0\pm1&0\\0\pm1&0&0\end{pmatrix}.$	$2\times3\times2^3=48$
Order of the matrix group:	96

a) $0=\begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix}$.

TABLE 4.10

Quartic Invariant Polynomials for Irreducible Representations *$\underline{X}$n , n=1,2,3,4.

Irrep.	Quartic invariant polynomial[a)]
*$\underline{X}$1,2	$\sum_{i=1}^{3}(\psi_i^4+\bar{\psi}_i^4)$
	$\sum_{i=1}^{3}\psi_i^2\bar{\psi}_i^2$
	$\sum_{i<j}(\psi_i^2\psi_j^2+\bar{\psi}_i^2\psi_j^2+\psi_i^2\bar{\psi}_j^2+\bar{\psi}_i^2\bar{\psi}_j^2)$
	$\sum_{i<j}\psi_i\bar{\psi}_i\psi_j\bar{\psi}_j$
	$\sum_{(ijk)}(\psi_i^2+\bar{\psi}_i^2)(\psi_j\bar{\psi}_j-\psi_k\bar{\psi}_k)$
*$\underline{X}$3,4	$\sum_{i=1}^{3}(\psi_i^4+\bar{\psi}_i^4)$
	$\sum_{i=1}^{3}\psi_i^2\bar{\psi}_i^2$
	$\sum_{i\neq j}\psi_i^2\bar{\psi}_j^2$
	$\sum_{i<j}\psi_i\bar{\psi}_i\psi_j\bar{\psi}_j$
	$\sum_{(ijk)}(\psi_i^2+\bar{\psi}_i^2)(\psi_j\bar{\psi}_j-\psi_k\bar{\psi}_k)$
	$\sum_{i<j}(\psi_i^2\psi_j^2+\bar{\psi}_i^2\bar{\psi}_j^2)$

a) (ijk) means cyclic permutation of (123).

TABLE 4.11

Quartic Invariant Polynomials for R-point Representations.

Irrep.	Quartic invariant polynomial
*R1	$\psi_1^4+\psi_2^4$, $\psi_1^2\psi_2^2$
*R2,3	$\psi_1^2\psi_2^2$
*R2◆*R3	$\psi_1^2\psi_2^2+\psi_3^2\psi_4^2-2\psi_1\psi_2\psi_3\psi_4$ $\psi_1^2\psi_4^2+\psi_2^2\psi_3^2+2\psi_1\psi_2\psi_3\psi_4$ $(\psi_1^2-\psi_3^2)\psi_2\psi_4+(\psi_2^2-\psi_4^2)\psi_1\psi_3$ $\psi_1^4+\psi_2^4+\psi_3^4+\psi_4^4+2(\psi_1^2\psi_3^2+\psi_2^2\psi_4^2)$
*R4	$\sum_{i=1}^{3}(\psi_i^4+\bar{\psi}_i^4)$ $\sum_{i=1}^{3}\psi_i^2\bar{\psi}_i^2$ $\psi_1^2\bar{\psi}_2^2+\psi_2^2\bar{\psi}_3^2+\psi_3^2\bar{\psi}_1^2$ $\bar{\psi}_1^2\psi_2^2+\bar{\psi}_2^2\psi_3^2+\bar{\psi}_3^2\psi_1^2$ $\sum_{i<j}(\psi_i^2\psi_j^2+\bar{\psi}_i^2\bar{\psi}_j^2)$ $\sum_{i<j}\psi_i\bar{\psi}_i\psi_j\bar{\psi}_j$

4.8. From the Molien function in Table 4.3 it can be seen that there are four independent quartic invariants. If we take basis functions as $\psi_1,\psi_2,\psi_3,\psi_4$, then these quartic invariants are given in Table 4.11.

The six dimensional representation *R4 is given in Table 4.9. This representation has six linearly independent quartic invariants (c.f. Table 4.3). Denoting basis functions as $\psi_1,\psi_2,\psi_3,\bar{\psi}_1,\bar{\psi}_2,\bar{\psi}_3$ we obtain these invariants as in Table 4.11.

Quartic invariants obtained in this Chapter we will use in Chapter 6 to construct Landau-Ginzburg-Wilson Hamiltonians for the renormalization-group treatment of structural phase transitions in A-15 systems.

CHAPTER 5

A Brief Introduction to the Renormalization-group and the ε-expansion

In order to analyze the possibility of second order structural phase transitions involving change of the unit cell in A-15 systems, we have applied the Landau theory of second order phase transitions (Chapter 2). One of the most serious limitations of that theory is the fact that possible fluctuations of the order parameter are neglected: sufficiently large fluctuations may, in principle,result in a first order phase transition which is otherwise prohibited by the Landau theory. Therefore, a theory which would take fluctuations of the order parameter into account must reduce to the Landau theory in the small fluctuations limit. Furthermore, conditions which appear in the Landau theory as necessary conditions for the phase transition to be of the second order, must remain in the "covering" theory as necessary conditions. Obviously, construction of such a"covering"theory is by no means unique.

In order to include fluctuations, Landau has suggested construction of an effective Hamiltonian which will depend upon a spatialy dependent order parameter $\psi(\underline{r})$.[40] This idea was first utilized by Landau and Ginzburg in their theory of superconductivity, and then developed by K.G.Wilson[41,42] in his Renormalization-group (RG) approach to the critical phenomena. There have already been several papers in which Wilson's method was appied to the investigation of second order structural phase transitions.[43,44] We will describe this method below.

Since we are investigating phenomena near the phase transition it is natural to assume that the only relevant part of the order parameter is its long-wavelength part:

$$\psi(\underline{r}) = \sum_{|\underline{k}|\leq k_0} (\psi'_{\underline{k}} + i\psi''_{\underline{k}}) e^{i\underline{k}\cdot\underline{r}} = \sum_{|\underline{k}|\leq k_0} \psi_{\underline{k}} e^{i\underline{k}\cdot\underline{r}} \quad , \qquad (5.1)$$

where k_0 is a cutoff wave number upon which critical properties should not depend.

The next step is to expand the effective Hamiltonian in $\psi(\underline{r})$ and its spatial derivatives. The Hamiltonian obtained in such a way, commonly called Landau-Ginzburg-Wilson Hamiltonian, must sutisfy all the symmetry requirements just as the Landau Free Energy. Thus we obtain:

$$H = -\int \{\tfrac{1}{2}(\nabla\psi)^2 + \tfrac{1}{2}u_0\psi^2 + u\psi^4\} dV \quad , \qquad (5.2)$$

where the integral is taken over the volume of the system. Near a phase transition u_0 and u are assumed to be analytic functions of thermodynamic variables (e.g., temperature, pressure,...).

A partition function Z is defined as a path integral:

$$Z=\int D(\psi)e^{H} \quad , \tag{5.3}$$

for which, neglecting fluctuations, we obtain the Landau Free Energy as a saddle point solution of the path integral.

The following step in the RG method is integrating out short wavelength degrees of freedom with $b^{-1}k_0<|\underline{k}|\leq k_0$ and b aconstant $b\gtrsim 1$. This"integrating out"is usually performed perturbatively (Feynman diagram techniques), where u is treated as a small parameter. Then a scale change is performed:

$$\underline{r}\rightarrow b\underline{r} \quad ,$$

$$\psi_{\underline{k}}\rightarrow\zeta\psi_{b\underline{k}} \quad . \tag{5.4}$$

The scale factor ζ in the order parameter is fixed such that a new effective Hamiltonian is obtained in the same form (5.2), neglecting higher order terms which arise:

$$H=\int\{\tfrac{1}{2}(\nabla\psi)^2+\tfrac{1}{2}u_0'\psi^2+u'\psi^4\}dV \quad . \tag{5.5}$$

The transformation H→H' is called a Renormalization-group transformation. It can be vewied as a transformation on the parameter space:

$$(u_0,u)\rightarrow(u_0',u') \quad . \tag{5.6}$$

This method exploits the fact that as the critical temperature is approached the only relevant length, which is a correlation length ξ, becomes infinite, and all physical properties become scale independent. Two systems connected by a RG transformation differ only in the scale, thus their free energies F and correlation lengths are related as:

$$F=b^{-3}F' \quad ,$$

$$\xi=b\xi' \quad . \tag{5.7}$$

From these relations it can be seen how important are,both, the fixed points of the RG transformation, defined by H=H', and the RG transformation itself in the neighbourhood of the fixed point (from which one is able to calculate critical exponents). Although this program looks simple, in practice it is not so. One reason is that: integrals which appear in the Feynman diagram expansion, as the critical temperature is approached, become divergent. In dimension d=3 it is impossible to extract the "most divergent" part. However, since it is possible to do so in dimension d=4, Wilson has suggested calculations should be done in the dimension $d=4-\varepsilon$, ε small (it turned out to be possible to define all of the appearing integrals for the noninteger dimensions). Then ε is the small parameter of the theory and all quantities are calculated to some order in ε (ε-expansion). Although this expansion is an asymptotic one,[45] in orer to estimate critical exponents, results are extrapolated to $\varepsilon=1$. This procedure in many cases gives good results when compared with other approximative methods and experiments.[46]

In the case of structural phase transitions one is considering a multicomponent order parameter $\psi_i(\underline{r})$, i=1,..., n, which belongs to a physically irreducible n-dimensional representation Γ of the high symmetry group G_0. The representation Γ must satisfy all the necessary conditions of the Landau theory. Therefore the Landau-Ginzburg-Wilson Hamiltonian is given as:

$$H=-\int\{\tfrac{1}{2}\sum_{i=1}^{n}(\nabla\psi_i)^2+\tfrac{1}{2}u_0\sum_{i=1}^{n}\psi_i^2+\sum_{j=1}^{m}u_jI_j\}dV\ , \qquad (5.8)$$

where I_j, $j=1,\ldots,m$, are all linearly independent Γ invariant polynomials quartic in the order parameter, and u_j, $j=0,\ldots,m$, are parameters forming an $(m+1)$-dimensional parameter space. Next,as discussed above, treating the quartic part of the Hamiltonian as of order one forms a RG transformation. Then one is aearching for the stable*) fixed points (to some order in ε) which correspond to second order phase transitions. Stability of a fixed point is determined from the linearized form of RG transformations in the neighborhood of the fixed point.

The method presented however does not predict low symmetry groups. In order to learn something about low symmetry groups one woul probably have to consider order parameter expectation values $\langle\psi_i\rangle$. Otherwise we consider groups allowed by the Landau theory and we disregard them if there is no stable fixed point present, and consider them allowed if there is a stable fixed point. In effect this represents analysis of the transition approaching it from above toward the transition point.

As a final part of this Chapter we will briefly describe a concrete application of Wilson's program to systems described by the Hamiltonian of Eq. 5.2.

Written in k-space the Hamiltonian is given as:

---

*)The fixed point is said to be stable iff there is a m-dimensional hypersurface (critical surface) in the (m+1)-dimensional parameter space, such that each point of the surface is transformed to the fixed point upon repeating RG transformation an infinite number of times.

$$H=-\tfrac{1}{2}\int_{\underline{k}}(k^2+u_0)\psi_{\underline{k}}\psi_{-\underline{k}}-u\int_{\underline{k}_1}\int_{\underline{k}_2}\int_{\underline{k}_3}\psi_{\underline{k}_1}\psi_{\underline{k}_2}\psi_{\underline{k}_3}\psi_{-\underline{k}_1-\underline{k}_2-\underline{k}_3}\ , \tag{5.9}$$

where

$$\int_{\underline{k}} \equiv (2\pi)^{-d}\int_{0\leq|\underline{k}|\leq k_0} d^d\underline{k} \quad . \tag{5.10}$$

This Hamiltonian can be written as a sum of two terms:

$$H=H_0+H_I \quad , \tag{5.11}$$

where the interaction Hamiltonian H_I is given as:

$$H_I=-u\int_{\underline{k}_1}\int_{\underline{k}_2}\int_{\underline{k}_3}\psi_{\underline{k}_1}\psi_{\underline{k}_2}\psi_{\underline{k}_3}\psi_{-\underline{k}_1-\underline{k}_2-\underline{k}_3} \quad . \tag{5.12}$$

A RG transformation is then defined as:

$$H'=\ln\{\int_{b^{-1}k_0<|\underline{k}|\leq k_0} D(\psi)\exp(H_0+H_I)\}\Big|_{\substack{\underline{k}\to b^{-1}\underline{k}\\ \psi_{\underline{k}}\to\zeta\psi_{b\underline{k}}}} \quad . \tag{5.13}$$

This path integral is evaluated by expanding the exponential, and treating H_I as a perturbation. The path integral becomes:

$$\int_{b^{-1}k_0<|\underline{k}|\leq k_0} D(\psi)e^{H_0}\sum_{j=0}^{\infty}H_I^j/j! \quad . \tag{5.14}$$

Therefore, evaluating the path integral (5.13) becomes equivalent to the evaluating correlation functions for the gaussian interaction H_0. Since the interaction H_I carries four fields, $\psi_{\underline{k}_1}$, $\psi_{\underline{k}_2}$, $\psi_{\underline{k}_3}$, $\psi_{\underline{k}_4}$, the j^{th} term in the expansion (5.14) is equivalent to the (4j-1)-correlation function for the gaussian Hamiltonian, where 1 is the number of fields whose momentum satisfies $|\underline{k}|\leq b^{-1}k_0$. On the other hand we know that for the gaussian Hamiltonian a correlation function is equal to the sum over all possible contractions. Each contraction $\overline{\psi_{\underline{k}}\psi_{\underline{k}}}$, gives a contribuition (called a propagator):

$$\overline{\psi_{\underline{k}}\psi_{\underline{k}'}} = (2\pi)^d \delta^d(\underline{k}+\underline{k}')/(k^2+u_0) \quad . \tag{5.15}$$

This procedure can be graphically expressed if we associate to $-H_I$ a vertex with four legs (Fig. 5.1). Four legs at the vertex represent four fields in H_I. Then path integral (5.14)

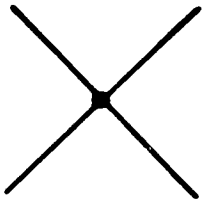

Figure 5.1

could be expresed as:

$$1-\bar{\Sigma}\times+\tfrac{1}{2}\bar{\Sigma}(\times\times)-(1/3!)\bar{\Sigma}(\times\times\times)+\ldots \quad , \tag{5.16}$$

where $\bar{\Sigma}$ means sum over all possible contractions. For example, for the first order terms we have:

$$\bar{\Sigma}\times = \times + 6 \, \text{} + 3 \, \text{} \quad , \tag{5.17}$$

where factors 6 and 3 come from topologically equivalent graphs, e.g.,

$$3 \, \text{  } = \text{} + \infty + \text{  } \quad . \tag{5.18}$$

Taking the logarithm of the expansion (5.16) is equivalent to removing of all disconnected graphs. Also,we are not interested in the graphs with no external legs (such as in Eq. 5.17), since these graphs give a constant contribution to H'. Therefore set of rules for computing any diagram is:[42]

(1) Label the momenta in the "incoming" sense at each vertex;

(2) Internal momenta range from $b^{-1}k_0$ to k_0, external

momenta range from 0 to $b^{-1}k_0$;

(3) Associate a propagator $(2\pi)^d\delta^d(\underline{k}+\underline{k}')/(k^2+u_0)$ with each internal line ($\underline{k}$ and $\underline{k}'$ are the two momentum labels on that line);

(4) Associate a factor $u(2\pi)^d\delta^d(\underline{k}_1+\underline{k}_2+\underline{k}_3+\underline{k}_4)$ with each vertex;

(5) Associate spin variable $\psi_{\underline{k}}=\zeta\psi'_{b\underline{k}}$ with each external leg.

(6) Integrate over internal and external momenta according to rule 2.

Thus, treatin coupling constant u as a small quantity we can determine a new Hamiltonian to some order in u. If we include all j-vertex diagrams we will obtain a new Hamiltonian up to j^{th} order in u.

In dimension d=4 we know only one fixed point, $H=H'=H^*$,

$$(u_0^*,u^*)=(0,0) \quad , \tag{5.19}$$

which we call gaussian fixed point. It turns out that we can consistently assume that in dimensions $d=4-\varepsilon$ there is besides gaussian fixed point another fixed point of order ε:

$$(u_0^*,u^*)=(O(\varepsilon),O(\varepsilon)) \quad . \tag{5.20}$$

Therefore expanding in powers of u is actually expanding in powers of ε. In order to obtain full ε-expansion we have to expand all integrals which appear in powers of ε (considering also u_0 to be of order ε)

According to the above, for example, u_0+k^2 is transformed as:

$$u_0+k^2\to b^{-d}\zeta^2\{u_0+6uA(u_0)\}+b^{-d-2}\zeta^2\{k^2-u^2B(k,u_0)\}. \tag{5.21}$$

Where $6uA(u_0)$ is a contribution from the graph of Fig.5.2,

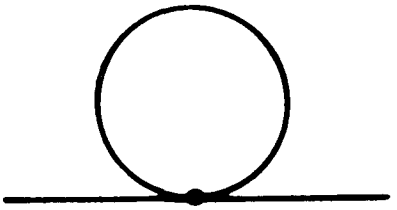

Figure 5.2

and $A(u_0)$ is given as:

$$A(u_0)=b^{-1}\int_{k_0<|\underline{k}|\leq k_0}(u_0+k^2)^{-1}=A(0)+u_0A'(0)+\ldots \quad (5.22)$$

(we will be especially interested in linear term in u_0

$$A'(0)=-K_4 \ln b \quad , \quad (5.23)$$

where K_4 is $(2\pi)^{-4}$ times the area of a three dimensional unit sphere), and $u^2B(k,u_0)$ represents a contribution from the

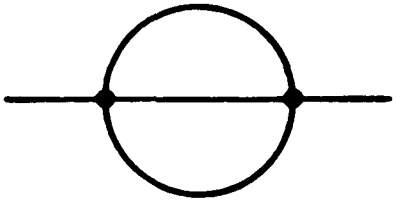

Figure 5.3

diagram of Fig. 5.3. $B(k,u_0)$ could be expanded in powers of k^2:

$$B(k,u_0)=B(0,u_0)+k^2B'(0,u_0)+\ldots \quad , \quad (5.24)$$

so that the coefficient of the k^2 in Eq. 5.21 is:

$$b^{-d-2}\zeta^2\{1-u^2B'(0,u_0)\}\simeq b^{-d-2}\zeta^2\exp\{-u^2B'(0,u_0)\}. \quad (5.25)$$

Since we need this coefficient to be unity, we have to choose ζ^2 as:

$$\zeta^2=b^{d+2}e^{u^2B'(0,u_0)} \quad . \quad (5.26)$$

On the other hand it could be shown[42] that critical exponent η*) is given as:

$$\eta=d+2-\frac{\ln(\zeta^*)^2}{\ln b} \quad , \tag{5.27}$$

where ζ^* is ζ evaluated at the fixed point. Therefore, critical exponent η is given to second order in ε as:

$$\eta=-u^2\,\frac{B'(0,0)}{\ln b} \quad . \tag{5.28}$$

With ζ^2 determined, the linear term in u_0 of the Eq. 5.21 to order ε is given as:

$$b^2 u_0\{1+6uA'(0)\}\simeq b^{2-6uK_4}u_0 \quad . \tag{5.29}$$

This linear term determines the critical exponent ν†) to order ε. In the neighbourhood of the fixed poin we can writte RG transformation fo u_0 as:

$$u_0'-u_0^*=\lambda_1(u_0-u_0^*)+\lambda_2(u-u^*) \quad , \tag{5.30}$$

where, to order ε, λ_1 is a coefficient of the linear term in u_0 given by Eq. 5.29:

$$\lambda_1\simeq b^{2-6u^*K_4} \quad . \tag{5.31}$$

Critical exponent ν is related to λ_1 as:[42]

$$\nu=\frac{\ln b}{\ln\lambda_1} \quad , \tag{5.32}$$

which in our case gives:

$$\nu=.5+1.5u^*K_4 \quad . \tag{5.33}$$

Critical exponent γ, which describes divergence of the "magnetic susceptibility" as the critical temperature

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*) The critical exponent η is defined through behaivor of the correlation function $\langle\psi(\underline{r})\psi(\underline{0})\rangle$ at the critical temperature $T=T_c$:

$$\langle\psi(\underline{r})\psi(\underline{0})\rangle_{T=T_c}\sim|\underline{r}|^{2-d-\eta} \quad .$$

†) The critical exponent ν is determined from divergence of a correlation length ξ as the critical temperature $T=T_c$ is approached:

$$\xi\sim|T-T_c|^{-\nu} \quad .$$

$T=T_c$ is approached, is given by the scaling law as:[47]

$$\gamma=\nu(2-\eta) \quad . \tag{5.34}$$

In order to calculate other critical exponents one must introduce a symmetry breaking field in the Hamiltonian, i.e., one has to introduce in the Hamiltonian term linear in the field ψ. This is not considered in this thesis.

CHAPTER 6

Application of Wilson's Method to Structural Phase Transitions in A-15 Systems[48]

Using a renormalization-group approach, as described in Chapter 5, we have treated structural phase transitions in the A-15 systems. The order parameter is taken to be of symmetry *R4, *X3, *X4, *X1, *X2 respectively. In chapter 4 we have obtained quartic invariants for these representations, which are needed for the construction of the corresponding Landau-Ginzburg-Wilson Hamiltonians. All results, presnted below, are obtained to order ε.

Representation *R4

In this case the quartic part of the Landau-Ginzburg-Wilson Hamiltonian, is

$$\sum_{i=1}^{6} v_i I_i \quad , \tag{6.1}$$

where v_i, i=1,...,6 are parameters and I_i, i=1,...,6 are all linearly independent quartic invariants of the *R4 representation, obtained in Chapter 4:

$$
\begin{aligned}
I_1 &= \sum_{i=1}^{3} (\psi_i^4+\bar{\psi}_i^4) \\
I_2 &= \sum_{i=1}^{3} \psi_i^2\bar{\psi}_i^2 \\
I_3 &= \psi_1^2\bar{\psi}_2^2+\psi_2^2\bar{\psi}_3^2+\psi_3^2\bar{\psi}_1^2 \\
I_4 &= \bar{\psi}_1^2\psi_2^2+\bar{\psi}_2^2\psi_3^2+\bar{\psi}_3^2\psi_1^2 \\
I_5 &= \sum_{i<j} (\psi_i^2\psi_j^2+\bar{\psi}_i^2\bar{\psi}_j^2) \\
I_6 &= \sum_{i<j} \psi_i\bar{\psi}_i\psi_j\bar{\psi}_j
\end{aligned}
\qquad (6.2)
$$

where ψ_1, ψ_2, ψ_3, $\bar{\psi}_1$, $\bar{\psi}_2$, $\bar{\psi}_3$ span representation *$\underline{R}$4. The RG equations for such a set of quartic invariants are:

$$
\begin{aligned}
u_0' &= b^{2-\eta}\{u_0+2(6v_1+v_2+v_3+v_4+2v_5)A(u_0)\}+O(\varepsilon^2) \\
v_1' &= b^{\varepsilon}\{v_1-\tfrac{1}{2}(72v_1^2+2v_2^2+2v_3^2+2v_4^2+4v_5^2)K_4 1nb\}+O(\varepsilon^3) \\
v_2' &= b^{\varepsilon}\{v_2-\tfrac{1}{2}(16v_2^2+48v_1v_2+8v_3v_5+8v_4v_5+2v_6^2)K_4 1nb\}+O(\varepsilon^3) \\
v_3' &= b^{\varepsilon}\{v_3-\tfrac{1}{2}(16v_3^2+48v_1v_3+8v_2v_5+8v_4v_5+v_6^2)K_4 1nb\}+O(\varepsilon^3) \\
v_4' &= b^{\varepsilon}\{v_4-\tfrac{1}{2}(16v_4^2+48v_1v_4+8v_2v_5+8v_3v_5+v_6^2)K_4 1nb\}+O(\varepsilon^3) \\
v_5' &= b^{\varepsilon}\{v_5-\tfrac{1}{2}(20v_5^2+48v_1v_5+4v_2v_3+4v_3v_4+4v_4v_2+v_6^2)K_4 1nb\}+ \\
&\quad O(\varepsilon^3) \\
v_6' &= b^{\varepsilon}v_6\{1-\tfrac{1}{2}(2v_6+16v_2+8v_3+8v_4+16v_5)K_4 1nb\}+O(\varepsilon^3),
\end{aligned}
\qquad (6.3)
$$

with

$$
A(u_0) = \int_{b^{-1}<|\underline{k}|\leq 1} (k^2+u_0)^{-1} \quad , \qquad (6.4)
$$

and where $b^{\varepsilon}\simeq 1+\varepsilon 1nb$; $K_d = 2^{-d+1}\pi^{-\frac{1}{2}d}\{\Gamma(\frac{1}{2}d)\}^{-1}$ is the surface area of a d-dimensional unit sphere, divided by $(2\pi)^d$. Factors $K_4 1nb$ come from the diagrams of Figure 6.1. However, diagrams shown on Figure 6.2 do not appear, since momentum is not conserved at vertex v_j.

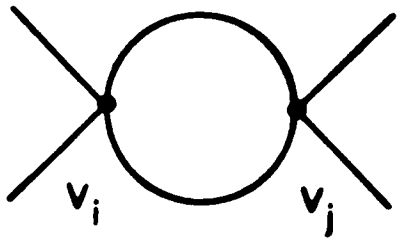

Figure 6.1

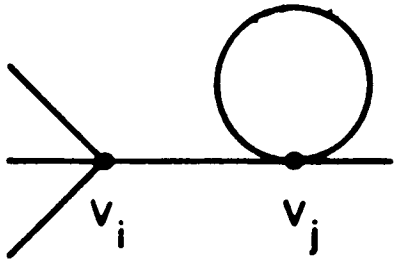

Figure 6.2

The critical exponent η is given to order ε^2 as:

$$\eta=\tfrac{1}{4}K_4^2(96v_1^2+v_2^2+v_3^2+v_4^2+v_5^2+2v_6^2) \quad , \qquad (6.5)$$

and comes from diagrams of Figure 6.3, which give contrib-

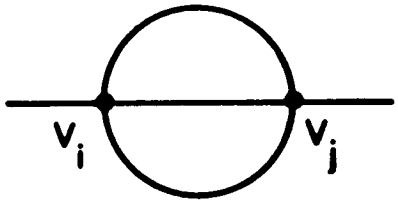

Figure 6.3

utions to the $\nabla\psi_i\cdot\nabla\psi_i$ term in the Hamiltonian. To order ε^2 there are no other diagrams contributing to this term. The exponent η then fixes the scaling factor ζ in such a way that the coefficient of the particular term $\nabla\psi_i\cdot\nabla\psi_i$ remains unchanged by renormalization-group equations.

Critical exponent ν is determined (cf. Eqs. 5.29-32)

from the linear term in u_0 of the $A(u_0)$ in the first equation of (6.3), i.e., from the diagrams of Fig. 6.4. This critical

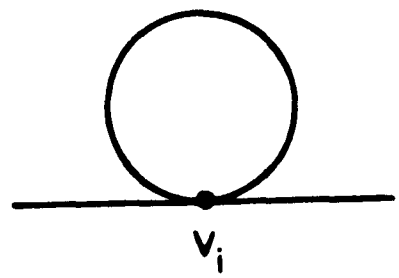

Figure 6.4

exponent is given to order ε as:

$$\nu^{-1}=2-2K_4(6v_1+v_2+v_3+v_4+2v_5)+0(\varepsilon^2) \quad . \tag{6.6}$$

These two critical exponents are to be calculated at the stable fixed point. The critical exponent γ is related to these two by the scaling law (5.34).

Since last six equations in (6.3) do not contain u_0, fixed poin may be evaluated by solving last six equations with $v_i'=v_i$, $i=1,\ldots,6$. After we introduce new variables

$$x_i=K_4v_i/\varepsilon \quad , \; i=1,\ldots,6 \quad , \tag{6.7}$$

we obtain set of six quadratic equations:

$$\begin{aligned}
x_1&=36x_1^2+x_2^2+x_3^2+x_4^2+2x_5^2\\
x_2&=8x_2^2+24x_1x_2+4x_3x_5+4x_4x_5+x_6^2\\
x_3&=8x_3^2+24x_1x_3+4x_2x_5+4x_4x_5+\tfrac{1}{2}x_6^2\\
x_4&=8x_4^2+24x_1x_4+4x_2x_5+4x_3x_5+\tfrac{1}{2}x_6^2\\
x_5&=10x_5^2+24x_1x_5+2x_2x_3+2x_3x_4+2x_4x_2+\tfrac{1}{2}x_6^2\\
x_6&=x_6(x_6+8x_2+4x_3+4x_4+8x_5) \quad .
\end{aligned} \tag{6.8}$$

These equations possess some apparent symmetry (e.g. x_3 and x_4 are equivalent; x_2, x_3 and x_4 are equivalent at $x_6=0$ etc.).

We find 24 real solutions of the equations (6.8) which

are tabulated in Table 6.1. However all of these solutions correspond to unstable fixed points. Therefore, according to Mukamel et al, we conclude that a second order transition, driven by the *R4 order parameter, is not permitted.

Representations *X3 and *X4

These two representations have six linearly independent quartic invariants, obtained in Chapter 4. The quartic part of the Hamiltonian is therefore given as:

$$\sum_{i=1}^{6} u_i J_i \quad , \tag{6.9}$$

where u_i, i=1,...,6 are parameters and the quartic invariants J_i, i=1,...,6 are given in Chapter 4 as:

$$\begin{aligned}
J_1 &= \sum_{i=1}^{3} (\psi_i^4 + \bar{\psi}_i^4) \\
J_2 &= \sum_{i=1}^{3} \psi_i^2 \bar{\psi}_i^2 \\
J_3 &= \sum_{i \neq j} \psi_i^2 \bar{\psi}_j^2 \\
J_4 &= \sum_{i<j} \psi_i \bar{\psi}_i \psi_j \bar{\psi}_j \\
J_5 &= \sum_{(ijk)} (\psi_i^2 + \bar{\psi}_i^2)(\psi_j \bar{\psi}_j - \psi_k \bar{\psi}_k) \\
J_6 &= \sum_{i<j} (\psi_i^2 \psi_j^2 + \bar{\psi}_i^2 \bar{\psi}_j^2) \quad ,
\end{aligned} \tag{6.10}$$

where $\sum_{(ijk)}$ is the sum over cyclic permutatins of the (123), and ψ_1, $\bar{\psi}_1$, ψ_2, $\bar{\psi}_2$, ψ_3, $\bar{\psi}_3$ are taken as the basis for either irreducible representation *X3 or *X4 (specific cases differ). For the special choice of the parameters, Hamiltonians of the representation *R4 and of the representations *X3 and *X4 have the same form. The correspondence is:

TABLE 6.1

Fixed Points for Irreducible Representation *R4.

Fixed point No.[a]	x_1	x_2	x_3	x_4	x_5	x_6
1	0	0	0	0	0	0
2	1/36	0	0	0	0	0
3	1/44	0	0	0	1/22	0
4	1/54	0	0	0	1/18	0
(5,6,7)[b]	1/72	1/12	0	0	0	0
(8,9,10)[b]	1/40	1/20	0	0	0	0
11	1/56	1/28	1/28	1/28	1/28	0
12	5/216	1/36	1/36	1/36	1/36	0
13	7/360	1/60	1/60	1/60	1/20	0
14	3/136	1/68	1/68	1/68	3/68	0
(15,16,17)[b]	1/54	1/18	1/36	1/36	1/36	0
(18,19,20)[b]	1/44	1/22	1/44	1/44	1/44	0
21	1/68	1/17	1/34	1/34	1/34	1/17
22	1/108	1/18	1/36	1/36	1/36	1/9
23	1/72	1/20	1/30	1/30	1/30	1/15
24	1/88	3/44	1/44	1/44	1/44	1/11

[a] Solutions $x_6=0$ agree with Ref.43

[b] For these fixed points permute x_2, x_3, x_4.

$$u_1 \leftrightarrow v_1$$
$$u_2 \leftrightarrow v_2$$
$$u_3 \leftrightarrow v_3 = v_4$$
$$u_4 \leftrightarrow v_6 \qquad (6.11)$$
$$u_5 = 0$$
$$u_6 \leftrightarrow v_5 \quad .$$

After introducing new variables x_i, $i=1,\ldots,6$ by the equations:

$$x_i = K_4 u_i/\varepsilon \quad , \quad i=1,\ldots,6 \quad , \qquad (6.12)$$

we obtain a set of fixed point equations:

$$\begin{aligned}
x_1 &= 36x_1^2+x_2^2+2x_3^2+x_5^2+2x_6^2 \\
x_2 &= 8x_2^2+x_4^2+6x_5^2+24x_1x_2+8x_3x_6 \\
x_3 &= 8x_3^2+\tfrac{1}{2}x_4^2+3x_5^2+24x_1x_3+4x_2x_6+4x_3x_6 \\
x_4 &= x_4^2-20x_5^2+8x_2x_4+8x_3x_4+8x_6x_4 \\
x_5 &= x_5(12x_1+6x_2+6x_3-5x_4+6x_6) \\
x_6 &= 10x_6^2+2x_3^2+\tfrac{1}{2}x_4^2+3x_5^2+24x_1x_6+4x_2x_3 \quad .
\end{aligned} \qquad (6.13)$$

There are some symmetries in these equations too (e.g., $x_5 \leftrightarrow -x_5$).

We have found 24 real solutions of equations (6.13), which we list in Table 6.2. First sixteen of them correspond to the sixteen fixed point solutions of the representation *R4, with $v_3 = v_4$.

In this case as well as in the previous one, we have found no stable fixed point solutions. Thus no second order phase transition, driven by the order parameter of the symmetry *X3 nor *X4 may occur.

Representations *X1 and *X2

We have found in Chapter 4 that these two represent-

TABLE 6.2

Fixed Points for Irreducible Representations *Xn, n=1,2,3,4.

Fixed point No.	x_1	x_2	x_3	x_4	x_5	x_6 [a]
1	0	0	0	0	0	0
2	1/36	0	0	0	0	0
3[a]	1/44	0	0	0	0	1/22
4[a]	1/54	0	0	0	0	1/18
5	1/72	1/12	0	0	0	0
6	1/40	1/20	0	0	0	0
7	1/56	1/28	1/28	0	0	1/28
8	5/216	1/36	1/36	0	0	1/36
9[a]	7/360	1/60	1/60	0	0	1/20
10[a]	3/136	1/68	1/68	0	0	3/68
11	1/54	1/18	1/36	0	0	1/36
12	1/44	1/22	1/44	0	0	1/44
13	1/68	1/17	1/34	1/17	0	1/34
14	1/108	1/18	1/36	1/9	0	1/36
15	1/72	1/20	1/30	1/15	0	1/30
16	1/88	3/44	1/44	1/11	0	1/44
17,18	3/176	5/88	5/176	-1/44	±1/88	5/176
19,20	7/432	1/24	5/144	-1/36	±1/72	5/144
21,22	1/144	1/24	1/48	-1/12	±1/24	1/48
23,24	1/80	3/40	1/80	-1/20	±1/40	1/80

[a] These rows and columns should be eliminated if one wants to read fixed points for irreducible representations *X1 and *X2.

ations both have five linearly independent quartic invariants, so the quartic part of the Hamiltonian is:

$$\sum_{i=1}^{5} w_i L_i \quad , \tag{6.14}$$

where w_i, i=1,...,5 are parameters, and L_i, i=1,...,5 are five linearly independent quartic invariants of the representations *X1 and *X2. These invariants have been given in Chapter 4 as:

$$\begin{aligned} L_1 &= \sum_{i=1}^{3} (\psi_i^4+\bar{\psi}_i^4) \\ L_2 &= \sum_{i=1}^{3} \psi_i^2\bar{\psi}_i^2 \\ L_3 &= \sum_{i<j} (\psi_i^2\psi_j^2+\psi_i^2\bar{\psi}_j^2+\bar{\psi}_i^2\psi_j^2+\bar{\psi}_i^2\bar{\psi}_j^2) \\ L_4 &= \sum_{i<j} \psi_i\bar{\psi}_i\psi_j\bar{\psi}_j \\ L_5 &= \sum_{(ijk)} (\psi_i^2+\bar{\psi}_i^2)(\psi_j\bar{\psi}_j-\psi_k\bar{\psi}_k) \quad , \end{aligned} \tag{6.15}$$

where ψ_1, $\bar{\psi}_1$, ψ_2, $\bar{\psi}_2$, ψ_3, $\bar{\psi}_3$ belong to a representation *X1 or *X2.

The Hamiltonian of this case becomes equivalent to the one for the representations *X3 and *X4, if we make correspondence:

$$\begin{aligned} w_1 &\leftrightarrow u_1 \\ w_2 &\leftrightarrow u_2 \\ w_3 &\leftrightarrow u_3 = u_6 \\ w_4 &\leftrightarrow u_4 \\ w_5 &\leftrightarrow u_5 \quad . \end{aligned} \tag{6.16}$$

This gives us twenty real fixed points given in the Table 6.2. Althou it was found in the previous case that all

of corresponding fixed point solutions are unstable, it does not imply that this is so in this case. However, calculatio has shown that, in this case too, all of the fixed points are unstable. Therefore we conclude that a second order phase transition is not allowed in this case either.

CHAPTER 7

Summary

To conclude this thesis we shall summarize the results obtained.

In Chapter 2 we found lower symmetry groups accesible by second order phase transitions driven by an order parameter of X- or R-point symmetry. Tables 2.1 to 2.3 summarize lower symmetry groups we have found. Precise comparison of our results with the experiments is possible only in a few known cases. However, in all cases in which transformation to a tetragonal symmetry group is observed, it is either found that the phase transition is first order, or (where there are insufficient data) it is found that the phase transition is "nearly first order". Therefore our results of Landau theory would imply either:a) there are possible second order transitions yet to be observed in experiments; or b) for these order parameters Landau theory is not applicable since large fluctuations prevent the phase transition from being second order. Our renormalization-group calculation favores the second possibility: we have found no stable fixed points.

Therefore we conclude that X- and R-point symmetry order parameters give us an example where second order phase transition is prevented by the large fluctuations of the order parameter. This conclusion dos not contradict experiments. All of the order parameters used in the RG analysis were six-dimensional, and we found no stable fixed points. It is interesting to note that in cases so far analyzed in the literature,[32] where multicomponent order parameter ($n \geq 4$) was considered, it turned out most of the times that no stable fixed point existed. Nonexistance of the stable fixed point was alwais attributed to the first order character of the phase transition. However, it is not the only possible explanation. for example a fixed point of order ε^{β}, $0<\beta<1$, would be missed by the ε-expansion. Furthermore, until more experimental data on multicomponent order parameters are available, we will not be able to evaluate the validity of our estimate obtained by ε-expansion with $\varepsilon=1$.

These are some of the questions which remain to be answered.

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Autobiographical Statement

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