Renormalization-group theory of structural phase transitions in A-15 compounds

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(Received 20 December 1977)

Hamiltonians of Landau-Ginzburg-Wilson type are constructed for order parameters which are bases for certain high-dimensional irreducible or physically irreducible representations in A-15 structure. These are all the representations with wave vectors Γ, X, and R and encompass cases of dimension 1, 2, 3, 4, and 6. A renormalization-group analysis was performed on each new distinct Hamiltonian using the Wilson-Fisher "ϵ expansion" method to order ϵ, in order to determine fixed points and stability, and critical exponents. For representations of R wave-vector symmetry, only the two-dimensional $R(1)$ has a stable fixed point and may produce a second-order phase transition; for all other R wave vector representations, fluctuations prevent second-order transition. No X point representation gives a second-order transition. Representations at Γ which are permitted to be second order by "Landau theory" remain so in this analysis. Generally, if the dimension of the representation is ≥ 4 the transition is not second order. Few experimental results are available for comparison: the known cases of Nb_3Sn and Nb_3Si agree with theory. A brief discussion is given of some possible reasons for absence of stable fixed points, i.e., a failure of the "ϵ expansion" in integral powers; letting $\epsilon \rightarrow 1$. A suggestion is made that a "hidden variable" may be present and may produce multicriticality owing to being accidentally set at a critical value in some samples.

I. INTRODUCTION

This paper reports the results of an investigation into the structural phase transition and related critical phenomena in systems known as "A-15 compounds." This class of compounds comprises a series of materials of composition A_3B where A is typically a transition metal (Nb, V, etc.) and B is an element of the IVth column (Sn, Si, Ge, . . . , etc.). The space group of the "A-15" compounds is $O_h^3 - Pn3m$. Among the reasons for considerable interest in this class of compounds is the occurrence of relatively high-temperature superconductivity in various members of this class.[1]

A structural instability or phase transition is observed in a large number of compounds. At a temperature T_m, the transition proceeds by transformation from space group O_h^3 to another lower-symmetry group. In the cases where the lower-symmetry structure space group is known, the transition is to a tetragonal symmetry group. Associated with this structural transition are a variety of elastic and electronic anomalies (softening of elastic coefficient, temperature-dependent magnetic susceptibility, etc.).

Since the discovery of the high-temperature superconductivity in these materials in 1954, and the discovery by Batterman and Barrett of the phase transition,[2] much work has been devoted to understanding the origin and interconnection of these phenomena. The phase transition has been ascribed by various authors to Jahn-Teller effect,[3] soft optical modes,[4] a "hidden" electronic order parameter,[5] charge-density waves,[6] coupled order parameters,[7] defects,[8] to name some recent proposals.

In a previous paper,[9] we reported the results of an investigation of possible lower-symmetry groups which could arise by second-order transition from the $O_h^3 - Pm3n$ group. That paper used the Landau thermodynamic theory of second-order phase transitions[10] and did not propose any physical identification of the order parameters. It utilized the possible symmetry of the order parameters taking them as bases for a single, physically irreducible representation of the group $O_h^3 - Pm3n$. Possible lower-symmetry phases were identified, which were compatible with second-order transition using allowable irreducible representations. It is known that such an analysis based on the Landau mean-field theory omits fluctuations of the order parameter and so can be considered a "small-fluctuation" limit of a more exact theory.[11]

The present paper continues our investigation of the structural phase transitions in A-15 systems. Here we use the modern renormalization-group methods pioneered by Kadanoff,[12] Wilson,[13] Fisher,[14] and others[15] to examine phase transitions driven by order parameters of high symmetry in these systems; the fluctuations are now included in the theory. We shall use the Wilson-Fisher "ϵ expansion" method[14]: we work to order ϵ. Since the method has been reviewed in many places[16] and applied in detail recently to some magnetic systems by Mukamel, Krinsky, and Bak,[17] we shall only give a sketch of our approach here.

The first step of the analysis is construction of the Landau-Ginzburg-Wilson (LGW) Hamiltonian.

Let the set of order parameters (fields) be denoted $\{\psi_\alpha^j\}$, $\alpha = 1, \ldots, n$ where $\{\psi_\alpha^j\} \rightarrow D^j$ and the D^j is a physically irreducible representation of the symmetry group $G (= O_h^3 - Pm3n)$. The $\{\psi_\alpha^j\}$ are bases for D^j. Since we shall restrict attention to one physically irreducible representation D^j at a time, we suppress index j in what follows. We construct all the linearly independent quartic (fourth-degree) invariants from the $\{\psi_\alpha\}$: denote these as $I_k(\{\psi_\alpha\})$, $k = 1, \ldots, m$. Denote the spatial gradient of ψ_α as $\nabla\psi_\alpha$. The Hamiltonian is then

$$\mathcal{H} = -\frac{1}{2}\int dV \sum_{\alpha=1}^{n} (r\psi_\alpha^2 + \nabla\psi_\alpha \cdot \nabla\psi_\alpha) - \int dV \sum_{k=1}^{m} u_k I_k . \tag{1}$$

The quantities $(r, u_1, u_2, \ldots, u_m)$ are parameters which are assumed to be analytic functions of the thermodynamic variables $(T, P, \ldots)$. By definition, each of the I_k is an absolute invariant under action of G. That is if $g \in G$

$$g\psi_\alpha(\vec{r}) = \psi_\alpha(g^{-1}\vec{r}) = \sum_\beta D(g)_{\beta\alpha}\,\psi_\beta(\vec{r}) \tag{2}$$

then

$$g I_k(\{\psi_\alpha(\vec{r})\}) = I_k(\{\psi_\alpha(g^{-1}\vec{r})\}) = I_k(\{\psi_\alpha(\vec{r})\}). \tag{3}$$

The partition function Z for such a system is obtained by performing the path integral

$$Z = \int \mathfrak{D}(\psi) e^{\mathcal{H}}. \tag{4}$$

Below we shall give the Hamiltonian, and renormalization-group analyses including search for fixed points and examination of stability for allowable order parameters belonging to physically irreducible representations labeled $^*R(q)$, $q = 1, \ldots, 4$; $^*X(s)$, $s = 1, \ldots, 4$; $^*\Gamma(t)$, $t = 1^\pm, \ldots, 5^\pm$, in the space group $G = O_h^3$.

Order parameters belonging to the R point are of interest since $^*R(4)$ is a six-dimensional irreducible representation—giving a six-component order parameter. This representation has also recently been utilized in an electronic model for properties of A-15 compounds.[18] $^*R(2) \oplus {}^*R(3)$ is a physically irreducible four-dimensional representation (direct sum of two complex-conjugate irreducible representations each of dimension 2). $^*R(1)$ is two dimensional. Of interest is that at R, $^*R = R$; only a single wave vector occurs in the star, so the above-mentioned are simultaneously irreducible ray representations of the factor (point) group $O_h^3/T = O_h$ and of the full space group O_h^3.

Representations at $^*X$ have been used by Gor'kov,[19] for an electronic model of A-15 properties, and at Γ have been used by Labbé Friedel.[3]

Of direct relevance to the present work is the current interest in analyses of critical behavior of systems described by order parameters of dimension $n \geq 4$. This was greatly stimulated by work of Mukamel *et al.*,[17] Aharony,[20] and others, with which we shall make some contact.

II. HAMILTONIAN FOR POINTS R, X, Γ

The first step in the construction of the LGW Hamiltonian for order parameters which are bases for space-group irreducible representations with wave vectors R, X, and Γ is to determine the number of independent "group invariant" polynomials which arise for each degree. The order parameters are taken here to span a physically irreducible representation of the space group so there exists a single bilinear Hermitian invariant form: the multiplicity is one. Because we are concerned with second-order phase transitions, we exclude order parameters for which a third-degree invariant exists.

To obtain the multiplicity of fourth- and higher-degree invariants, we have calculated the Molien generating function for each of the irreducible representations we use. Elsewhere,[21] we presented the Molien function for all irreducible representations going with R, X, and Γ wave vectors: inspection of this function gives the number $C_{4,1} = m$.

To obtain the actual invariants we use a projection operator.[22] The particular structure of the invariants, but not the multiplicity of distinct ones, depends upon the specific form chosen for the representation. We used the Kovalev generating matrices in our work, which fixes the "gauge"; all the details needed for complete specification of the images of the irreducible (or physically irreducible) representations were given in a previous publication.[9c]

We remark that in the present work we limit ourselves to G-invariant Hamiltonians up to and including only polynomials of fourth degree (quadrilinear real form in the order parameters); this is conventional in most of the current work using "ϵ-expansion" methods. Thus, the structure of the Hamiltonians with which we are concerned is always that of Eq. (1). In what follows here, we present the results of determination of the structure and number (m) of quartic invariants for irreducible representations with wave vectors R, X, and Γ.

$^*R(j) = R(j)$ representations

Recall the space group is $O_h^3 - Pm3n$. For wave vector $R = (\pi/a, \pi/a, \pi/a)$, one finds the translation

TABLE I. Invariant quartic polynomials for R-point representations.

Representation	
$R(1)$	$\psi_1^4+\psi_2^4;\quad \psi_1^2\psi_2^2$
$R'(2)$	$\psi_1^2\psi_2^2+\psi_3^2\psi_4^2-2\psi_1\psi_2\psi_3\psi_4$
	$\psi_1^2\psi_4^2+\psi_2^2\psi_3^2+2\psi_1\psi_2\psi_3\psi_4$
	$\psi_1^4+\psi_2^4+\psi_3^4+\psi_4^4+2(\psi_1^2\psi_3^2+\psi_2^2\psi_4^2)$
	$(\psi_1^2-\psi_3^2)\psi_2\psi_4+(\psi_2^2-\psi_4^2)\psi_1\psi_3$
$R(4)$	$\sum_{i=1}^{3}(\psi_i^4+\overline{\psi}_i^4)$
	$\sum_{i=1}^{3}\psi_i^2\overline{\psi}_i^2$
	$\psi_1^2\overline{\psi}_2^2+\psi_2^2\overline{\psi}_3^2+\psi_3^2\overline{\psi}_1^2$
	$\overline{\psi}_1^2\psi_2^2+\overline{\psi}_2^2\psi_3^2+\overline{\psi}_3^2\psi_1^2$
	$\sum_{i<j}[\psi_i^2\psi_j^2+\overline{\psi}_i^2\overline{\psi}_j^2]$
	$\sum_{i<j}\psi_i\overline{\psi}_i\psi_j\overline{\psi}_j$

TABLE II. Invariant quartic polynomials for X-point representations.[a]

Representation	Invariant quartic polynomial[b]
$X(1)$	$\sum_{i=1}^{3}(\psi_i^4+\overline{\psi}_i^4)$
	$\sum_{i=1}^{3}\psi_i^2\overline{\psi}_i^2$
	$\sum_{i<j}(\psi_i^2\psi_j^2+\psi_i^2\overline{\psi}_j^2+\overline{\psi}_i^2\psi_j^2+\overline{\psi}_i^2\overline{\psi}_j^2)$
	$\sum_{i<j}\psi_i\overline{\psi}_i\psi_j\overline{\psi}_j$
	$\sum_{(ijk)}(\psi_i^2+\overline{\psi}_i^2)(\psi_j\overline{\psi}_j-\psi_k\overline{\psi}_k)$

[a] $X(1)$ given in this table and remaining $X(j)$, $j=2$, 3, 4 see text.

[b] (ijk) means cyclic permutation of (123).

group of R to be the entire (primitive) Bravais cubic group; thus, the star of R comprises only the vector R. The little point group of R is then $Pm3n/T=m3n=O_h$, the full octahedral point group. The allowable physically irreducible ray representations for this case are denoted $R(1)$, $R'(2)=R(2)\oplus R(3)$, $R(4)$ by Miller and Love[23]; dimensions of these are 2, $4=2+2$, and 6. The four-dimensional one is the direct sum of complex conjugate irreducible representations. Noteworthy is the six-dimensional irreducible representation $R(4)$; it is the highest (single group) *local* degeneracy permitted in any of the 230 crystallographic space groups.

In Table I, we present a listing of the fourth-degree invariant polynomials[22] for each of these representations: basis functions $\{\psi_\alpha\}$ always refer to the indicated representation D only.

A. *X(j) = X(j) representations

For wave vector $X_1=(\pi/a,0,0)$, the little point group is $G(X_1)/T=D_{4h}$. The star consists of the three wave vectors $*X=\{X_1, X_2, X_3\}$ which involve cyclic permutation of x, y, and z. Allowable irreducible ray representations of the little group D_{4h} are all two dimensional. Hence, the space-group irreducible representations, which are induced from the irreducible representations of $G(X_1)$ to the full group are six dimensional. These four irreducible representations are denoted $X(j)$, $j=1,2,3,4$.

We can observe now that as matrix groups, $X(1)$ and $X(2)$ are "quasiequivalent" (we first learned of this terminology from L. Michel). That is, a similarity transformation by a fixed matrix will transform $X(1)$ into $X(2)$ and *vice versa*. Technically this is an *outer* automorphism since $X(1)$ and $X(2)$ are inequivalent irreducible representation of O_h^3. Quasiequivalence has the obvious consequence that the Molien functions are identical. In Table II quartic invariants are given: there are five such linearly independent ones.

Likewise $X(3)$ and $X(4)$ are quasiequivalent; and in fact, also quasiequivalent to $R(4)$. In Table I, the six linearly independent quartic invariants of each is given.

We note that representations $X(1)$ and $X(2)$ (present notation) were used by Gor'kov[19] in his theory of the properties of A-15 compounds.

B. *Γ(j) = Γ(j) representations

At wave vector $\Gamma=(0,0,0)$, the little point group is again (as at R) $Pm3n/T=O_h$. Now the irreducible representations needed are the vector representations of O_h: there are ten of them: $j=1\pm$, ..., $5\pm$. These representations have been used in earlier work, in which a Jahn-Teller mechanism was examined,[3] soft phonons were proposed,[4] and a Landau thermodynamic theory of the cubic-tetragonal phase was considered.

As mentioned earlier, we shall only carry out the analyses for order parameters belonging to irreducible representations which satisfy the Landau (stability) criterion. In case of Γ, these

TABLE III. Invariant quartic polynomials for Γ-point representations.[a]

Representation	Invariant quartic polynomial
Γ1−	ψ^4
Γ3−	$(\psi_1^2+\psi_2^2)^2$
Γ4−	$(\psi_1^2+\psi_2^2+\psi_3^2)^2$ $\psi_1^4+\psi_2^4+\psi_3^4$

[a] For the remaining $\Gamma(j)$ see text.

exclude all irreducible representations except the following "active" ones (using the notation of Miller and Love[23]):

$$\Gamma1-;\ \Gamma2\pm;\ \Gamma3-;\ \Gamma4-;\ \Gamma5\pm.$$

The quasiequivalent representations are Γ1− and Γ2±; Γ4− and Γ5±. Thus, in Table III, quartic invariants are given for the three *not* quasiequivalent irreducible representations. Note that only Γ4− (Γ5±) has two linearly independent quartic invariants; the others have only one.

III. RENORMALIZATION GROUP EQUATION AND FIXED POINTS

We begin with the six-dimensional, quasiequivalent representations $R(4), X(3), X(4)$. For these representations, the ϵ-expansion gives renormalization-group (RG) equations, which to order ϵ, are:

$$\begin{aligned}
r' &= b^2[r+2(6u_1+u_2+u_3+u_4+2u_5)A(r)]+O(\epsilon^2),\\
u_1' &= b^\epsilon[u_1-\tfrac{1}{2}(72u_1^2+2u_2^2+2u_3^2+2u_4^2+4u_5^2)\\
&\quad\times K_4\ln b]+O(\epsilon^3),\\
u_2' &= b^\epsilon[u_2-\tfrac{1}{2}(16u_2^2+48u_1u_2+8u_3u_5\\
&\quad+8u_4u_5+2u_6^2)K_4\ln b]+O(\epsilon^3),\\
u_3' &= b^\epsilon[u_3-\tfrac{1}{2}(16u_3^2+48u_1u_3+8u_2u_5\\
&\quad+8u_4u_5+u_6^2)K_4\ln b]+O(\epsilon^3),\\
u_4' &= b^\epsilon[u_4-\tfrac{1}{2}(16u_4^2+48u_1u_4+8u_2u_5\\
&\quad+8u_3u_5+u_6^2)K_4\ln b]+O(\epsilon^3),\\
u_5' &= b^\epsilon[u_5-\tfrac{1}{2}(20u_5^2+48u_1u_5+4u_2u_3\\
&\quad+4u_2u_4+4u_3u_4+u_6)K_4\ln b]+O(\epsilon^3).\\
u_6' &= b^\epsilon u_6[1-\tfrac{1}{2}(2u_6+16u_2+8u_3\\
&\quad+8u_4+16u_5)K_4\ln b]+O(\epsilon^3).
\end{aligned}\tag{5}$$

In Eq. (5),

$$A(r)=\int_{b^{-1}<|k|\le 1}(k^2+r)^{-1}\,d^dk \tag{6}$$

and $b^\epsilon\approx 1+\epsilon\ln b$; $(2\pi)^dK_d$ is the surface area of a $(d-1)$-dimensional unit sphere.

Since the last six equations in (5) do not contain r, the fixed point may be evaluated by solving these equations with $u_i'=u_i$. After we introduce new variables x_i, $i=1,\ldots,6$,

$$x_i=K_4u_i/\epsilon,\quad i=1,\ldots,6, \tag{7}$$

we obtain a set of six quadratic equations:

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

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 Eq. (8) which are tabulated in Table IV. However, all of these solu-

TABLE IV. Fixed points for the representations $R(4)$, $X(j)$, $j=1,\ldots,4$.

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

[a] These are obtained by cyclic permutation of x_2, x_3, x_4.

[b] Solutions $x_6=0$ agree with Mukamel's type-I antiferromagnets with magnetization orthogonal to the wave vector (Ref. 18).

TABLE V. Fixed points for the representation $R'(2)$ of the group O_h^3.

Fixed point no.	x_1	x_2	x_3	x_4
1	0	0	0	0
2	0	0	$\frac{1}{40}$	0
3	$\frac{1}{24}$	$\frac{1}{24}$	$\frac{1}{48}$	0
4; $\lambda \in [-1,1]$ [a]	$\frac{1}{20}(1+\frac{1}{2}\lambda)$	$\frac{1}{20}(1-\frac{1}{2}\lambda)$	$\frac{1}{80}$	$\pm\frac{1}{2}(1-\lambda^2)^{1/2}$

[a]The appearance of this line of fixed points is discussed in Ref. 24.

tions correspond to unstable fixed points. Therefore, we conclude that a second-order transition driven by $R(4)$, $X(3)$, $X(4)$ order parameters, is not permitted.

Next we consider the quasiequivalent, six-dimensional representations $X(1)$ and $X(2)$. The quartic part of the Hamiltonian for these representations is given in Table II. After a simple "gauge" transformation

$$\begin{aligned} &\psi_i \to (1/\sqrt{2})(\psi_i + \bar{\psi}_i), \\ &\bar{\psi}_i \to (1/\sqrt{2})(\psi_i - \bar{\psi}_i), \end{aligned} \quad i = 1,2,3 \tag{9}$$

it can be seen that parameter space of this case is the same as a hypersurface of the previous case with $u_6 = 0$. Some of the previous solutions, which lie on this surface might turn out, in principle, to have only one unstable direction perpendicular to the surface. Such fixed points would become stable on the surface. However, this does not happen in our case, so that $u_6 = 0$ fixed points are still unstable: there cannot be a second-order phase transition driven by an order parameter of symmetry $X(1)$ and $X(2)$.

Next, we consider four-dimensional representation $R'(2)$ whose quartic part of the Hamiltonian is given in Table I. After introducing new variables x_i defined as in Eq. (7) with $i = 1, \ldots, 4$, we obtain the fixed-point equations as:

$$\begin{aligned} x_1 &= 10x_1^2 + 2x_2^2 + 4x_4^2 + 24x_1x_3 + 8x_2x_3 - 4x_1x_2, \\ x_2 &= 10x_2^2 + 2x_1^2 + 4x_4^2 + 24x_2x_3 + 8x_1x_3 - 4x_1x_2, \\ x_3 &= x_1^2 + x_2^2 + 40x_3^2 + \tfrac{1}{2}x_4^2, \\ x_4 &= 8x_1x_4 + 8x_2x_4 + 16x_3x_4. \end{aligned} \tag{10}$$

We find real solutions of these equations, given in Table V. All of these solutions correspond to unstable fixed points and we conclude that order parameters of symmetry $R'(2)$ cannot drive a second-order phase transition.

Three-dimensional quasiequivalent representations $\Gamma 4-$ and $\Gamma 5\pm$ give quartic portion of the Hamiltonians as in Table III. This type of LGW Hamiltonian has been analyzed by Aharony[20] and

TABLE VI. Fixed points for the representations $\Gamma 4-$ and $\Gamma 5+$ of the group O_h^3.

Fixed point no.	x_1	x_2
1	0	0
2	0	$\frac{1}{36}$
3	$\frac{1}{44}$	0
4	$\frac{1}{36}$	$-\frac{1}{108}$

others. A change of variables as in Eq. (7) gives fixed points of Table VI. To order ϵ only fixed point No. 3 is stable giving critical exponent (to order ϵ at $\epsilon = 1$)

$$\nu = \tfrac{27}{44} \cong 0.614. \tag{11}$$

Two-dimensional representation $R(1)$ reduces also to the case discussed by Wilson and Fisher.[14] The fixed points obtained are tabulated in Table VII (after usual change of variables). To order ϵ all fixed points, except fixed point No. 3 are unstable. The stable fixed point gives critical exponent

$$\nu = \tfrac{3}{5} = 0.6. \tag{12}$$

Another two-dimensional representation is $\Gamma 3-$. There are two fixed points for this representation:

$$x = 0 \quad \text{and} \quad x = \tfrac{1}{40}. \tag{13}$$

The second fixed point is stable giving the same critical exponent as in the previous case.

Finally, one-dimensional quasiequivalent representations $\Gamma 1-$, $\Gamma 2\pm$ also have only one stable fixed point

$$x = \tfrac{1}{36}, \tag{14}$$

which gives exponent

$$\nu = \tfrac{7}{12} \cong 0.583. \tag{15}$$

IV. ANALYSIS OF RESULTS

It is interesting to compare the results obtained by the present RG analysis with results obtained

TABLE VII. Fixed points for the representation $R(1)$ of the group O_h^3.

Fixed point no.	x_1	x_2
1	0	0
2	0	$\frac{1}{36}$
3	$\frac{1}{44}$	0
4	$\frac{1}{24}$	$-\frac{1}{36}$

by the use of the Landau theory of second-order phase transitions. For R-point representations, we have found here that *only* the representation $R(1)$ produces a stable fixed point. Therefore, we conclude that in the other cases $R'(2)$ and $R(4)$, fluctuations prevent the phase transition from being second order. For the $R(1)$ representation we have already found allowable low-symmetry groups,[9] but no experimental observations have yet been reported of a structural phase transition from higher-symmetry group O_h^3 to a lower-symmetry group with change of the size of the unit cell equal in all three directions. We predict for such a transition (if observed), on the basis of the present calculation, that the divergence of the specific heat C_p at the transition temperature, will be described by a critical exponent

$$\alpha = 0.1 \,. \tag{16}$$

For all X-point representations, we have found no stable fixed points, so we conclude that no second-order structural phase transition driven by an X-point order parameter may occur, due to the large fluctuations of the order parameter.

$\Gamma-$ point order parameters have been previously analyzed[9] by the Landau theory. Here we find that fluctuations do not change character of the phase transition: phase transitions to low-symmetry groups remain second order. We find critical exponents α to be:

$$\alpha = \tfrac{1}{22} \cong 0.045 \quad \text{for irreducible representations } \Gamma 4-, \Gamma 5\pm, \tag{17}$$

$$\alpha = 0.1 \quad \text{for irreducible representation } \Gamma 3-, \tag{18}$$

$$\alpha = \tfrac{1}{6} \cong 0.17 \quad \text{for irreducible representations } \Gamma 1-, \Gamma 2\pm. \tag{19}$$

Differences between α's for different representations are quite large (~ 50%) so we believe it should be possible to distinguish them experimentally. At present, it has not been determined whether the observed phase transitions are second order. In most cases, it is believed the transition is "nearly second" order. Two experimentally lower-symmetry groups have been reported to date.

(a) In the case of Nb_3Sn it is found[25] that the low-symmetry group is D_{4h}^9 and that the transition is first order. Since this transition does not involve a change of the unit cell, it could be driven only by a $\Gamma-$ point order parameter. However Landau theory has already shown[9] that the transition $O_h^3 \to D_{4h}^9$ (with no change in unit cell) is not allowed as a second-order transition and thus the result agrees with experiment.

(b) The second case is Nb_3Si,[26] which has low-symmetry group C_{4h}^4 (doubling in x and y directions). This transition could be driven by X-point order parameter (M-point order parameters would also produce doubling in x and y directions, but the symmetry subgroup would then be nonprimitive). However for X-point, it has been shown[9] using Landau theory that this subgroup is not allowed as second order. This agrees with the experimental report.[26]

The nonexistence of a stable fixed point is interpreted as signifying absence of a second-order phase transition. However, a stable fixed point may be missed by the ϵ expansion in integral powers: the leading power may be a noninteger. There is also a problem of a general nature in our procedure of taking $\epsilon = 1$ at the end of the calculation. Such a large ϵ can even produce a change in stability of a fixed point by going to higher order in the expansion. Here, we assume that the conclusions regarding fixed points and their stability near $\epsilon = 0$ could be extrapolated, but there is question regarding the accuracy of other results obtained by setting $\epsilon = 1$.

From our results it is apparent that many representations were eliminated as bases for allowable order parameters of second-order phase transitions, because of nonexistence of a stable fixed point. In the framework of these calculations, we conclude that transitions associated with such representations are multicritical. This is not in contradiction with experimental results, which show that only some of the samples undergo structural phase transition: the coupling parameters of the LGW Hamiltonian may depend upon some as yet unknown, or hidden, thermodynamic variables. Such variables may be accidentally set at a critical value for transforming samples. One possibility which has been suggested is the concentration, or distribution of vacancies[8]; but a recent determination of structure and electron-charge distribution in V_3Si by accurate x-ray diffraction measurements appears to find in this sample neither the suggested concentration of vacancies, nor the suggested ordered distribution.[27] If there is some additional variable, it would be interesting to have it identified and controlled experimentally.

ACKNOWLEDGMENTS

This work was supported in part by NSF Grant DMR 76-20641-A01 and FRAP-City University of New York 11680. This work was based in part on a thesis submitted to Physics Department, The City College, City University of New York (by M.V.J.), in partial fulfillment of the requirements for the degree of Ph.D. in Physics.

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