Continuous solid-solid phase transitions driven by an eight-component order parameter: Hamiltonian densities and renormalization-group theory

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Continuous solid-solid phase transitions driven by an eight-component order parameter are investigated. We list the active eight-dimensional physically irreducible representations we find among the 230 crystallographic space groups and the matrix images onto which they map the symmetry operations. We obtain the Landau potential (to fourth degree) as well as the Landau-Ginzburg-Wilson Hamiltonian for each case. We obtain the recursion relations in renormalization-group (RG) theory, and calculate the fixed points. We find that none of the fixed points are stable. Thus for transitions driven by an eight-component order parameter, none can be continuous according to RG theory.

Theoretical descriptions of continuous (second-order) transitions between two solid phases have been of considerable interest for many years. The Landau theory[1,2] is a mean-field approach which imposes group-theoretical restrictions on the transition. When critical fluctuations are taken into account, the renormalization-group (RG) theory[3] imposes additional conditions. In both theories, the transition is driven by an n-component order parameter. Cases for $n \leq 6$ have previously been considered.[4–6] In this paper, we consider the case $n=8$. We restrict our attention to commensurate phases with symmetry among the 230 crystallographic space groups. We find that none of the possible transitions driven by an eight-component order parameter are allowed to be continuous in RG theory.

Consider a possible transition from a phase of space-group symmetry G_0 to a phase of space-group symmetry G. Landau theory requires that G be a subgroup of G_0 and that the transition be driven by an order parameter $\boldsymbol{\phi}$, which is an n-component vector in the carrier space of an active physically irreducible representation (irrep) of G_0. The irrep consists of a mapping of space-group elements onto a set of n-dimensional orthogonal matrices called the *image* of the irrep. The irrep is "active"[2] if these matrices satisfy both the Landau[7] and Lifshitz[8] conditions (a requirement of Landau theory, if the transition is to be continuous).

The Landau potential is obtained by constructing invariant polynomials in the components of $\boldsymbol{\phi}$. To fourth degree, the potential can be written

$$V=\frac{r}{2}\boldsymbol{\phi}\cdot\boldsymbol{\phi}+P_4(\boldsymbol{\phi}) \ , \tag{1}$$

where

$$P_4=\sum_{\nu=1}^{p} u_\nu I_\nu(\boldsymbol{\phi}) \ . \tag{2}$$

The functions $I_1, I_2, \ldots, I_p$ are linearly independent fourth-degree polynomials which are each invariant under every matrix operation in the image. The coefficients r and u_ν are arbitrary and carry the temperature and pressure dependence of the potential. Within Landau theory, allowed continuous transitions to lower-symmetry phases G are found by minimizing V for all possible ranges of values of the coefficients u_ν.

We find that there are only nine active eight-dimensional irreps ($n=8$) among all the irreps of the 230 space groups. These map space-group elements onto only four distinct images (see Table I). The labeling of irreps in Table I follows the convention of Miller and Love. The fourth-degree invariants listed in Table I are given explicitly in Table II. (Tolédano and Tolédano[9] reported *five* eight-dimensional active images. We believe their fifth image M_5 is in error. We do not find any irrep of $P6_3mc$ to be eight dimensional. Also, they only give five invariant polynomials for M_3 and six for M_4, in disagreement with our results.) Minimization of V for these cases would yield continuous phase transitions allowed by Landau theory.

In RG theory, the Landau-Ginzburg-Wilson (LGW) Hamiltonian H is constructed by adding isotropic gradient terms to the Landau potential:[3]

$$H=\sum_{i=1}^{n}(\nabla\phi_i)^2+\frac{r}{2}\boldsymbol{\phi}\cdot\boldsymbol{\phi}+P_4(\boldsymbol{\phi}) \ . \tag{3}$$

The coupling coefficients u_ν in P_4 form a p-dimensional vector $\mathbf{u}$ in "coupling-coefficient space," and the polynomial $P_4(\mathbf{u})$ is now considered to be a function of position in that space. As the critical point is approached, $\mathbf{u}$ "flows" towards a stable fixed point $\mathbf{u}^*$. The flow of $\mathbf{u}$ is

TABLE I. The images of the eight-dimensional active irreps and their fourth-degree invariant polynomials.

Image	Active irreps	Invariants
M_1	L_3^+, L_3^- of O_h^7	I_1,I_2,I_3,I_4,I_5
M_2	L_3 of T_d^2 and L_3^+, L_3^- of O_h^5	I_1,I_2,I_3,I_4,I_5,I_6
M_3	$L_2^+\oplus L_3^+, L_2^-\oplus L_3^-$ of T_h^4	$I_1,I_2,I_3,I_4,I_5,I_7,I_8$
M_4	$L_2^+\oplus L_3^+, L_2^-\oplus L_3^-$ of T_h^3	$I_1,I_2,I_3,I_4,I_5,I_6,I_7,I_8$

TABLE II. The invariant fourth-degree polynomials of the components of the order parameter $\boldsymbol{\phi}=(\eta_1,\zeta_1,\eta_2,\zeta_2,\eta_3,\zeta_3,\eta_4,\zeta_4)$.

$$I_1=(\eta_1^2+\zeta_1^2+\eta_2^2+\zeta_2^2+\eta_3^2+\zeta_3^2+\eta_4^2+\zeta_4^2)^2$$

$$I_2=(\eta_1^2+\zeta_1^2)^2+(\eta_2^2+\zeta_2^2)^2+(\eta_3^2+\zeta_3^2)^2+(\eta_4^2+\zeta_4^2)^2$$

$$I_3=[(\eta_1^2-\zeta_1^2)+(\eta_2^2-\zeta_2^2)][(\eta_3^2-\zeta_3^2)+(\eta_4^2-\zeta_4^2)]+4[(\eta_1^2-\zeta_1^2)(\eta_2^2-\zeta_2^2)+(\eta_3^2-\zeta_3^2)(\eta_4^2-\zeta_4^2)]$$
$$-2\sqrt{3}(\eta_1\zeta_1-\eta_2\zeta_2)[(\eta_3^2-\zeta_3^2)-(\eta_4^2-\zeta_4^2)]-2\sqrt{3}(\eta_3\zeta_3-\eta_4\zeta_4)\,[(\eta_1^2-\zeta_1^2)-(\eta_2^2-\zeta_2^2)]+12(\eta_1\zeta_1+\eta_2\zeta_2)(\eta_3\zeta_3+\eta_4\zeta_4)$$

$$I_4=[(\eta_1^2-\zeta_1^2)+(\eta_2^2-\zeta_2^2)][(\eta_3^2-\zeta_3^2)+(\eta_4^2-\zeta_4^2)]+\tfrac{16}{3}(\eta_1\zeta_1\eta_2\zeta_2+\eta_3\zeta_3\eta_4\zeta_4)$$
$$+\tfrac{4}{3}(\eta_1\zeta_1+\eta_2\zeta_2)(\eta_3\zeta_3+\eta_4\zeta_4)+\frac{2}{\sqrt{3}}(\eta_1\zeta_1-\eta_2\zeta_2)[(\eta_3^2-\zeta_3^2)-(\eta_4^2-\zeta_4^2)]+\frac{2}{\sqrt{3}}(\eta_3\zeta_3-\eta_4\zeta_4)[(\eta_1^2-\zeta_1^2)-(\eta_2^2-\zeta_2^2)]$$

$$I_5=(\eta_1\zeta_1+\eta_2\zeta_2)[(\eta_3^2+\zeta_3^2)+(\eta_4^2+\zeta_4^2)]+(\eta_3\zeta_3+\eta_4\zeta_4)[(\eta_1^2+\zeta_1^2)+(\eta_2^2+\zeta_2^2)]$$
$$-2[\eta_1\zeta_1(\eta_2^2+\zeta_2^2)+\eta_2\zeta_2(\eta_1^2+\zeta_1^2)]-2[\eta_3\zeta_3(\eta_4^2+\zeta_4^2)+\eta_4\zeta_4(\eta_3^2+\zeta_3^2)]+\sqrt{3}[(\eta_1^2-\eta_2^2)(\eta_3^2-\eta_4^2)-(\zeta_1^2-\zeta_2^2)(\zeta_3^2-\zeta_4^2)]$$

$$I_6=3(\eta_1\eta_2\eta_3\eta_4+\zeta_1\zeta_2\zeta_3\zeta_4)+\eta_1\eta_2\zeta_3\zeta_4+\eta_1\zeta_2\eta_3\zeta_4+\eta_1\zeta_2\zeta_3\eta_4+\zeta_1\eta_2\eta_3\zeta_4+\zeta_1\eta_2\zeta_3\eta_4+\zeta_1\zeta_2\eta_3\eta_4$$

$$I_7=[(\eta_1^2-\zeta_1^2)+(\eta_3^2-\zeta_3^2)][(\eta_2^2-\zeta_2^2)+(\eta_4^2-\zeta_4^2)]-\frac{2}{\sqrt{3}}[(\eta_1^2-\zeta_1^2)-(\eta_3^2-\zeta_3^2)](\eta_2\zeta_2-\eta_4\zeta_4)$$
$$-\frac{2}{\sqrt{3}}[(\eta_2^2-\zeta_2^2)-(\eta_4^2-\zeta_4^2)](\eta_1\zeta_1-\eta_3\zeta_3)+\tfrac{4}{3}(\eta_1\zeta_1+\eta_3\zeta_3)(\eta_2\zeta_2+\eta_4\zeta_4)+\tfrac{16}{3}(\eta_1\zeta_1\eta_3\zeta_3+\eta_2\zeta_2\eta_4\zeta_4)$$

$$I_8=(\eta_1^2-\eta_3^2)[(\eta_2^2+\zeta_2^2)-(\eta_4^2+\zeta_4^2)]+(\eta_2^2-\eta_4^2)(\zeta_1^2-\zeta_3^2)-3(\zeta_1^2-\zeta_3^2)(\zeta_2^2-\zeta_4^2)\;+\frac{8}{\sqrt{3}}[\eta_1\eta_3(\eta_1\zeta_3+\eta_3\zeta_1)+\eta_2\eta_4(\eta_2\zeta_4+\eta_4\zeta_2)]$$
$$-\frac{4}{\sqrt{3}}[\eta_1\eta_2(\eta_1\zeta_2+\eta_2\zeta_1)+\eta_3\eta_4(\eta_3\zeta_4+\eta_4\zeta_3)+\eta_1\eta_4(\eta_1\zeta_4+\eta_4\zeta_1)+\eta_2\eta_3(\eta_2\zeta_3+\eta_3\zeta_2)]\;+4(\eta_1\zeta_1-\eta_3\zeta_3)(\eta_2\zeta_2-\eta_4\zeta_4)$$

TABLE III. The recursion relations for the image M_4.

$$du_1/d\ln\lambda=\epsilon u_1-(\tfrac{8}{3}u_1^2+\tfrac{4}{3}u_1u_2+\tfrac{8}{3}u_3^2+\tfrac{8}{27}u_4^2+\tfrac{1}{4}u_5^2+\tfrac{1}{16}u_6^2+\tfrac{4}{3}u_3u_7+\tfrac{4}{27}u_4u_7+\tfrac{8}{27}u_7^2-\tfrac{4}{3}u_3u_8+\tfrac{4}{9}u_4u_8+\tfrac{1}{2}\sqrt{\tfrac{1}{3}}u_5u_8+\tfrac{7}{9}u_8^2)$$

$$du_2/d\ln\lambda=\epsilon u_2-(2u_1u_2+\tfrac{5}{3}u_2^2-\tfrac{2}{3}u_3^2-\tfrac{2}{27}u_4^2+\tfrac{1}{8}u_5^2-\tfrac{1}{16}u_6^2-\tfrac{1}{3}u_3u_7-\tfrac{1}{27}u_4u_7-\tfrac{2}{27}u_7^2+\tfrac{1}{3}u_3u_8-\tfrac{1}{9}u_4u_8+\tfrac{1}{4}\sqrt{\tfrac{1}{3}}u_5u_8+\tfrac{1}{18}u_8^2)$$

$$du_3/d\ln\lambda=\epsilon u_3-(2u_1u_3+\tfrac{2}{3}u_2u_3-\tfrac{1}{6}u_3^2+\tfrac{1}{3}u_3u_4+\tfrac{1}{18}u_4^2-\tfrac{1}{16}u_5^2+\tfrac{1}{48}u_6^2+\tfrac{1}{6}u_3u_7+\tfrac{1}{6}u_4u_7$$
$$+\tfrac{1}{2}\sqrt{\tfrac{1}{3}}u_5u_7+\tfrac{1}{18}u_7^2+\tfrac{1}{6}u_2u_8+2u_3u_8-\tfrac{1}{9}u_4u_8-\tfrac{1}{8}\sqrt{3}u_5u_8+\tfrac{11}{18}u_7u_8-\tfrac{17}{36}u_8^2)$$

$$du_4/d\ln\lambda=\epsilon u_4-(\tfrac{3}{2}u_3^2+2u_1u_4+\tfrac{2}{3}u_2u_4+u_3u_4-\tfrac{1}{18}u_4^2+\tfrac{9}{16}u_5^2+\tfrac{1}{16}u_6^2+\tfrac{7}{6}u_3u_7+\tfrac{5}{18}u_4u_7$$
$$-\tfrac{1}{2}\sqrt{\tfrac{1}{3}}u_5u_7+\tfrac{1}{6}u_7^2-\tfrac{1}{6}u_2u_8-\tfrac{4}{3}u_3u_8-\tfrac{1}{9}u_4u_8-\tfrac{1}{8}\sqrt{\tfrac{1}{3}}u_5u_8-\tfrac{11}{18}u_7u_8-\tfrac{1}{12}u_8^2)$$

$$du_5/d\ln\lambda=\epsilon u_5-(2u_1u_5+u_2u_5-u_3u_5+u_4u_5-\tfrac{1}{3}u_5u_7-4\sqrt{\tfrac{1}{3}}u_3u_8+\tfrac{4}{3}\sqrt{\tfrac{1}{3}}u_4u_8+\tfrac{2}{3}u_5u_8+\tfrac{8}{3}\sqrt{\tfrac{1}{3}}u_8^2)$$

$$du_6/d\ln\lambda=\epsilon u_6-(2u_1u_6+\tfrac{8}{3}u_3u_6+\tfrac{8}{9}u_4u_6+\tfrac{8}{9}u_6u_7)$$

$$du_7/d\ln\lambda=\epsilon u_7-(2u_1u_7+\tfrac{2}{3}u_2u_7-\tfrac{2}{3}u_3u_7-\tfrac{2}{9}u_4u_7-\sqrt{\tfrac{1}{3}}u_5u_7-\tfrac{2}{9}u_7^2-\tfrac{1}{3}u_2u_8-\tfrac{11}{3}u_3u_8+\tfrac{1}{9}u_4u_8+2\sqrt{\tfrac{1}{3}}u_5u_8-\tfrac{11}{9}u_7u_8+\tfrac{5}{3}u_8^2)$$

$$du_8/d\ln\lambda=\epsilon u_8-(\sqrt{\tfrac{1}{3}}u_5u_7+2u_1u_8+u_2u_8+3u_3u_8-\tfrac{1}{3}u_4u_8+\sqrt{\tfrac{1}{3}}u_5u_8+u_7u_8-\tfrac{2}{3}u_8^2)$$

TABLE IV. Fixed points $\mathbf{u}^* = (u_1, u_2, u_3, u_4, u_5, u_6, u_7, u_8)$ and eigenvalues of the matrix $(\partial\beta_\nu/\partial u_{\nu'})$ evaluated at the fixed points.

Fixed points	Eigenvalues
$\epsilon(0,0,0,0,0,0,0,0)$	$\epsilon(-1,-1,-1,-1,-1,-1,-1,-1)$
$\epsilon(\frac{3}{8},0,0,0,0,0,0,0)$	$\epsilon(1,-\frac{1}{4},-\frac{1}{4},-\frac{1}{4},-\frac{1}{4},-\frac{1}{4},-\frac{1}{4},-\frac{1}{4})$
$\epsilon(0,\frac{3}{5},0,0,0,0,0,0)$	$\epsilon(1,-\frac{1}{5},-\frac{3}{5},-\frac{3}{5},-\frac{2}{5},-1,-\frac{3}{5},-\frac{2}{5})$
$\epsilon(\frac{3}{16},\frac{3}{8},0,0,0,0,0,0)$	$\epsilon(\frac{1}{8},1,-\frac{3}{8},-\frac{3}{8},-\frac{1}{4},-\frac{5}{8},-\frac{3}{8},-\frac{1}{4})$
$\epsilon(\frac{3}{8},-\frac{3}{32},\frac{3}{64},\frac{9}{64},0,\frac{3}{4},0,0)$	$\epsilon(1,\frac{1}{8},-\frac{5}{8},-\frac{3}{8},-\frac{3}{8},-\frac{1}{4},-\frac{3}{8},-\frac{1}{4})$
$\epsilon(\frac{3}{8},-\frac{3}{32},\frac{3}{64},\frac{9}{64},0,-\frac{3}{4},0,0)$	$\epsilon(1,\frac{1}{8},-\frac{5}{8},-\frac{3}{8},-\frac{3}{8},-\frac{1}{4},-\frac{3}{8},-\frac{1}{4})$
$\epsilon(\frac{3}{10},-\frac{3}{20},\frac{3}{40},\frac{9}{40},0,\frac{6}{5},0,0)$	$\epsilon(1,-\frac{1}{5},-1,-\frac{3}{5},-\frac{3}{5},-\frac{2}{5},-\frac{3}{5},-\frac{2}{5})$
$\epsilon(\frac{3}{10},-\frac{3}{20},\frac{3}{40},\frac{9}{40},0,-\frac{6}{5},0,0)$	$\epsilon(1,-\frac{1}{5},-1,-\frac{3}{5},-\frac{3}{5},-\frac{2}{5},-\frac{3}{5},-\frac{2}{5})$

determined by p recursion relations which take the form,

$$\frac{d\mathbf{u}}{d\ln\lambda} = \boldsymbol{\beta}(\mathbf{u}) \ . \tag{4}$$

Critical properties are obtained from stable fixed points as $\lambda \to \infty$. A fixed point $\mathbf{u}^*$ satisfies the p nonlinear equations

$$\beta_\nu(\mathbf{u}^*) = 0 \ , \tag{5}$$

and will be stable if in addition all of the eigenvalues of the matrix $(\partial\beta_\nu/\partial u_{\nu'})$ are positive at the fixed point. To one-loop order, we can write[10]

$$\boldsymbol{\beta} = \epsilon\mathbf{u} - \tfrac{3}{2}\mathbf{u}\wedge\mathbf{u} \ , \tag{6}$$

where the symmetric product $\mathbf{u}\wedge\mathbf{u}$ is given by

$$P_4(\mathbf{u}\wedge\mathbf{u}) = \frac{1}{144}\sum_{i,k}\left[\frac{\partial^2 P_4(\mathbf{u})}{\partial\phi_i\phi_k}\right]^2 \ . \tag{7}$$

The polynomial resulting from the summation can be decomposed into a linear combination of the invariants I_ν, the coefficients of which form the vector $\mathbf{u}\wedge\mathbf{u}$ in the coupling-coefficient space.

The eight recursion relations which arise for image M_4 are given in Table III. The recursion relations which arise for the other images can easily be obtained by simply setting some of the coefficients u_ν to zero. For example, the five recursion relations for image M_1 are obtained from Table III by setting $u_6 = u_7 = u_8 = 0$.

Fixed points are found by setting the right-hand side of each recursion relation equal to zero, and solving the resulting p nonlinear equations. We have searched by computer for solutions of these equations and found eight fixed points (Table IV). From the eigenvalues in Table IV, we see that none of these fixed points are stable for any of the images under consideration. Of course, we cannot *guarantee* that we have found *all* of the fixed points. However, our search was thorough, so we are fairly confident that we have found all of the fixed points and that no stable fixed point exists for these images.

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