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Tricritical Exponents and Scaling Fields

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The tricritical behavior of a classical three-well-potential model for two-component systems (such as He³-He⁴ mixtures) is discussed by using renormalization-group techniques. The tricritical exponents and scaling fields are calculated for three dimensions.

A model for a two-component system with a tricritical point (such as in He³-He⁴ mixtures) is found to show molecular-field tricritical behavior (apart from logarithmic corrections). The model can be viewed as a generalization of the model of Blume, Emery, and Griffiths (BEG).¹ It is solved in three dimensions by using Wilson's approximate renormalization-group recursion relations.² The recursion relations were previously shown to give nonclassical behavior for ordinary critical points.²⁻⁶ The tricritical transition differs from an ordinary second-order transition by the existence of an additional density with critical fluctuations.^{7,8} The tricritical scaling fields are also evaluated. They are the field variables in which the thermodynamic and correlation functions are scaling invariant.^{7,9}

We propose a model that exhibits a first-order, second-order, or tricritical phase transition depending on the value of an external nonordering field g .⁸ Let $s(\vec{R})$ denote a classical Ising spin of range $-\infty < s < +\infty$ at site \vec{R} of a discrete cubic lattice; and let $\vec{\delta}$ denote all nearest-neighbor lattice vectors. Then we consider a system with the Hamiltonian $-\mathcal{H}/k_B T \equiv H = H_{\text{ex}} + H_{\text{pot}}$, in which the exchange-interaction term and the potential-energy term are given by

$$H_{\text{ex}} = J' \sum_{\vec{R}, \vec{\delta}} s(\vec{R}) s(\vec{R} + \vec{\delta}), \quad (1a)$$

and

$$H_{\text{pot}} = - \sum_{\vec{R}} [r' s^2(\vec{R}) + u' s^4(\vec{R}) + v' s^6(\vec{R})] \quad (1b)$$

with the coefficients r' , u' , and v' depending on the temperature T , nonordering field g , and strength of the tricritical interaction [compare Eqs. (3) and (5)].

The *Ansatz* for the potential-energy term H_{pot} can be justified either by starting from a tricritical Landau-Ginzberg form¹⁰ for $H\{s\}$ or by replacing the BEG spin-1 model for He³-He⁴ mixtures¹ by a continuous-spin model with a spin-weight factor. From both approaches one expects a tricritical transition to occur for some H_{pot} consisting of the sum of three-well potentials at each lattice site \vec{R} (in contrast to two-well potentials for ordinary second-order transitions²). In fact, the renormalization scheme yields this result for the potential at the tricritical point (T_t, g_t) as shown in Fig. 1. For fixed $g < g_t$ the side wells of the potential dominate and we expect the model to exhibit a second-order transition at a temperature $T_c(g)$, whereas for $g > g_t$ we expect a first-order transition at $T_1(g)$. The three-well potential simulates the competition between two densities, one of which is the ordering density m as in ordinary critical phenomena, and the other is an additional nonordering

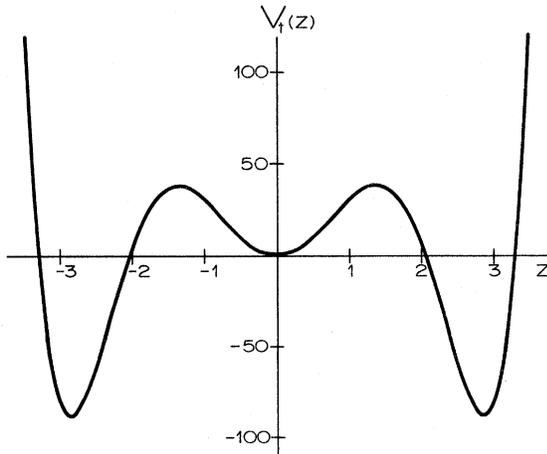


FIG. 1. Plot of the tricritical three-well potential $V_t = Q_p/v_p$, defined by Eq. (5), versus the reduced spin variable z .

density n .⁸ As in the BEG model, the densities m and n can be represented by

$$m = \langle s \rangle, \quad n = 1 - \langle s^2 \rangle. \quad (2)$$

Thus, an ordering field contribution to the Hamiltonian (1) has the form $H_h = h \sum_{\vec{R}} s(\vec{R})$, whereas nonordering field effects are included in the quadratic term of Eq. (1b)

On expanding $s(\vec{R} + \vec{\delta})$ to quadratic order in $\vec{\delta}$, replacing the \vec{R} summation by an \vec{x} integration, and substituting $s(\vec{x}) = (d/\bar{q}J')^{1/2} z(\vec{x})$ (where d and \bar{q} denote the respective dimension and coordination numbers of the lattice), we obtain from Eq. (1) a reduced Hamiltonian H_0 of the general form²³

$$H_p = - \int d^3x \left[\frac{1}{2} |\nabla z(\vec{x})|^2 + Q_p \{ z(\vec{x}) \} \right], \quad (3a)$$

$$Q_p(z) = r_p z^2 + u_p z^4 + v_p z^6 + \dots, \quad (3b)$$

with, for $p=0$, the initial values¹¹ $r_0 = d(r'/\bar{q}J' - 1)$, $u_0 = (d/\bar{q}J')^2 u'$, and $v_0 = (d/\bar{q}J')^3 v'$.

We use the renormalization-group method to discuss the tricritical properties of model (1) in *three* dimensions. To calculate the partition function $Z = \text{Tr} \exp(H_0)$ near a critical point, Wilson² has introduced an integration scheme over shells of successively decreasing momenta. At each stage the form of the Hamiltonian is required to remain invariant. In particular, the effective Hamiltonians (3) for spin fluctuations of wave vector $|\vec{q}| < 2^{-p}$ (with p an integer) are determined by the approximate recursion relations²

$$Q_{p+1}(z) = -2^d \ln [I_p(2^{1-d/2} z) / I_p(0)], \quad (4a)$$

$$I_p(z) = \int_{-\infty}^{+\infty} dy \exp \left[-y^2 - \frac{1}{2} Q_p(z+y) - \frac{1}{2} Q_p(z-y) \right]. \quad (4b)$$

At a critical point the correlation length of spin fluctuations becomes infinite, i.e., small momenta dominate, and the series Q_p is expected to approach a "fixed point" $Q^*(z)$ as $p \rightarrow \infty$. All critical properties can be determined from the eigenfunctions and eigenvalues of Eqs. (4) linearized about $Q^*(z)$.²⁴

We find a tricritical fixed point Q_t^* of the Hamiltonian H_0 in Eq. (3) by starting from a set of nonzero, initial constants $r_0, u_0, v_0 \ll 1$. On expanding the non-Gaussian terms under the integral in Eq. (4), we obtain by induction recursion relations for the quantities r_p, u_p , and v_p , with $p > 0$. These equations can be solved for dimension $d=3$. The solutions to order v_p^2 vary slowly with p and are small compared to 1, which indicates their consistency. For large p the recursion relations yield to leading order¹²

$$Q_p(z) \approx v_p (z^6 - 15z^4 + 45z^2), \quad (5a)$$

$$v_p \approx v_0 / (1 + 450 v_0 p). \quad (5b)$$

The potential Q_p/v_p is plotted in Fig. 1 and has the form anticipated for a tricritical phase transition. In the limit $p \rightarrow \infty$ the result (5) approaches $Q_t^* = 0$, which we call the "Gaussian tricritical fixed point."

We find that this fixed point corresponds to a tricritical phase transition characterized by *two* relevant densities and leads to molecular-field tricritical exponents (apart from logarithmic corrections¹³) in three dimensions. In contrast, the Gaussian fixed point for ordinary critical points gives molecular-field behavior in greater than four dimensions, where it describes the critical behavior even of non-Gaussian models.²³ The evaluation of the molecular-field tricritical exponents and scaling fields for our model is summarized below and leads to the results listed in Table I.

The linearization of the recursion relations in $\delta Q = Q - Q_t^*$ about a fixed point Q_t^* leads to $\delta Q_{p+1}(2^{d/2-1} z) = \hat{L}(Q_t^*) \delta Q_p(z)$, with a linear operator \hat{L} determined by Eqs. (4). For $Q_t^* = 0$ the operator \hat{L} reduces to \hat{L}_0 defined by

$$\begin{aligned} \hat{L}_0 Q_p(z) &= 2^{-d} \pi^{-1/2} \int_{-\infty}^{+\infty} dy e^{-y^2} \\ &\quad \times \left[\frac{1}{2} Q_p(z+y) + \frac{1}{2} Q_p(z-y) \right] \\ &= 2^{-d} \exp \left(\frac{1}{4} \partial^2 / \partial z^2 \right) Q_p(z). \end{aligned} \quad (6)$$

Here the last equality is obtained by expanding Q_p in powers of y and evaluating the integrals. Hence, the linearized recursion relations (4a)

TABLE I. Tricritical exponents in the Gaussian approximation.

| (k, l) | $\dot{\nu}_t \dot{x}_{kl}$ | $\dot{\nu}_t [d - 2\dot{x}_{kl}]$ | $\dot{\nu}_t [d - \dot{x}_{kl}]$ | $d/\dot{x}_{kl} - 1$ | $2[1 + \dot{x}_{kl} - 1/2d]$ |
|----------|----------------------------|--|----------------------------------|--------------------------|------------------------------|
| (0, 1) | $\dot{\beta}_t = 1/4$ | $\dot{\gamma}_t = 1$ | $\dot{\Delta}_t = 5/4$ | $\dot{\delta}_t = 5$ | $\dot{\eta}_t = 0^a$ |
| (1, 0) | $\dot{\omega}_t = 1/2^b$ | $\dot{\lambda}_t = \dot{\alpha}_t = 1/2^b$ | 1^c | $\dot{\delta}_{n,t} = 2$ | $\dot{\eta}_{n,t} = 1$ |
| (2, 0) | 1 | -1/2 | $\dot{\phi}_t = 1/2^b$ | 1/2 | 3 |

^aThe value $\dot{\eta}_t = 0$ is enforced by the approximations made to derive Eqs. (4).

^bThe exponents $\dot{\omega}_t$, $\dot{\lambda}_t$, and $\dot{\phi}_t$ were defined in Ref. 1.

^cThis result follows from the condition $\dot{\nu}_t [d - \dot{x}_{10}] = 1$; hence $\dot{\nu}_t = 1/2$, $\dot{\Delta}_{n,t} = 1$, and $\dot{\omega}_t + \dot{\lambda}_t = 1$.

and (6) are equivalent to the eigenvalue problem⁴

$$\hat{L}_0 \hat{Q}(z) = 2^{\dot{\beta}} \hat{Q}(2^{d/2-1} z), \quad \hat{Q}_p = 2^{p\dot{\beta}} \hat{Q}. \quad (7)$$

We call the eigenfunctions \hat{Q} of this equation *scaling densities* and the exponents $\dot{\beta}$ *scaling indices* of the system. All quantities are tricritical quantities; a subscript t is suppressed for simplicity.

The solution of the eigenvalue problem (7) for dimension $d = 3$ yields

$$\hat{Q}_{kl}(z) = H_{2k+l}(z/\sqrt{2}), \quad (8)$$

$$\dot{Y}_k = 3 - (k + \frac{1}{2}l). \quad (9)$$

Here H_{2k+l} denotes the Hermite polynomials (the index l is restricted to $l = 0, 1$ and k is a positive integer). Thus the degree of \hat{Q}_{kl} in z is $2k + l$. The scaling densities differ by their symmetry properties. For example, \hat{Q}_{01} corresponds to the ordering density m , \hat{Q}_{10} to the nonordering density n and simultaneously to the energy density. The quartic term in the potential-well model gives rise to a contribution to the scaling density \hat{Q}_{20} in the Hamiltonian. This term competes with the exchange term (1a). Therefore, it determines the critical line and hence defines the tricritical crossover exponent $\dot{\phi}_t$.⁷ Both scaling densities \hat{Q}_{10} and \hat{Q}_{20} are relevant, i.e., exhibit critical fluctuations. This fact represents the principal difference between the transitions corresponding to the *tricritical* Gaussian fixed point (5) and the ordinary second-order Gaussian fixed point. Hence the tricritical point can be characterized as the *simultaneous* instability point of the system to *two* types of critical fluctuations. Corrections to the molecular-field tricritical behavior due to scaling densities of higher order ($k > 2$) will be discussed in a separate paper. It is found that the asymptotic tricritical form of some thermodynamic functions is not a power law but a power law multiplied by a fractional

power of a logarithm.¹³

The scaling indices $\dot{\beta}$ in Eq. (9) measure the sensitivity of the system to fluctuations in the corresponding scaling density \hat{Q} . If $\hat{Q}(\vec{R})$ scales like $|\vec{R}|^{-\dot{x}}$ in the sense of the Kadanoff operator algebra,^{14,15} then the indices \dot{x} and $\dot{\beta}$ are related by $\dot{\beta} = d - \dot{x}$. Equation (9) and this relation yield for $d = 3$ the tricritical exponents summarized in Table I, where both their operator-algebra notation and Greek-alphabet notation is given. The results agree with tricritical exponents that have been calculated by conventional mean-field approximation.^{1,16} The exponents are independent of the spin dimensionality, i.e., are the same for an n -vector model.¹³ All exponent relations following from a tricritical scaling theory⁷ are satisfied, for example, $\dot{\omega}_t = \dot{\lambda}_t / (\dot{\delta}_{n,t} - 1) = 1 - \dot{\alpha}_t$ and $\dot{\lambda}_t = (2 - \dot{\eta}_{n,t})\dot{\nu}_t$. The exponents are also consistent with the tricritical exponents found for He³-He⁴ mixtures. Furthermore, we expect that for the model the critical-line exponents $\alpha, \beta, \gamma, \dots$ are the exponents of the three-dimensional Ising model.¹⁷

The concept of *scaling fields* was introduced in a scaling approach to tricritical phase transition.⁷ It proves crucial for a scaling-invariant definition of the departure of a system from criticality. (In general terms the problem is to define a thermodynamic field space with a metric determined by the nature of the phase transition itself.)

From this viewpoint it is important to calculate *microscopically* the scaling fields in which the thermodynamic and correlation functions are homogeneous functions. These fields are not necessarily the experimental deviating fields, for example, $\delta T = (T - T_t)/T_t$, $\delta g = (g - g_t)/g_t$, etc.

Here we propose a method to calculate the scaling fields. Writing the effective Hamiltonian H_0 of Eq. (3) in terms of the scaling densities \hat{Q}_{kl} , we obtain

$$Q_{p=0} = \sum_{k=1}^3 \mu_{k,0}^{(0)} \hat{Q}_{k,0}, \quad (10)$$

with the "fields" μ given by

$$\begin{aligned}\mu_{1,0}^{(0)} &= \frac{1}{2}(r_0 + 6u_0 + 45v_0), \\ \mu_{2,0}^{(0)} &= \frac{1}{4}(u_0 + 15v_0), \quad \mu_{3,0}^{(0)} = \frac{1}{8}v_0.\end{aligned}\quad (11)$$

By using renormalization-group ideas it has been generally shown⁹ that the thermodynamic potential of the system is a homogeneous function of the fields μ defined by Eq. (10). These fields variables are "conjugate" to the scaling densities \hat{Q} . Therefore, they can be identified with the scaling fields introduced in the tricritical scaling approach.

The tricritical point (T_t, g_t) is defined by the condition that all scaling fields μ conjugate to densities \hat{Q} with $\dot{y} > 0$ vanish. Hence the two conditions $\mu_{1,0}^{(0)} = \mu_{2,0}^{(0)} = 0$ define the tricritical field values T_t and g_t in terms of the model parameters. Expanding the results (11) about the tricritical point, we obtain relations between the scaling fields and experimental fields,

$$\mu_{1,0} = c_{1,T} \delta T + c_{1,g} \delta g, \quad \mu_{2,0} = c_{2,T} \delta T, \quad (12)$$

where we retained only terms linear in δT and δg .

In the tricritical scaling theory⁷ the critical line is determined by $\mu_{1,c} = r_c \mu_{2,c}^{1/\hat{q}_t}$. (A similar relation holds for the first-order transition line.) Hence, it approaches the tricritical point in the (μ_1, μ_2) plane tangentially parallel to the μ_2 axis. This is generally not the case for the critical line expressed in terms of the experimental fields in the $(\delta T, \delta g)$ plane, where using Eq. (12), we obtain $\delta_c T \propto \delta_c g$. In this sense the scaling fields μ are also the "singled-out fields" of Griffiths and Wheeler.¹⁸ Furthermore, this example shows explicitly that the tricritical exponents as discussed here are defined relative to these particular reference fields. (We always use a fluxion dot to denote quantities in the scaling field space.)

The conceptual difference between scaling fields and experimental fields^{4,15} can be formulated in terms of a "relativity hypothesis" for critical points: *All phase transitions determine a frame of reference of scaling fields. Critical exponents are defined relative to this frame of scaling fields and determine the homogeneity properties of thermodynamic and correlation functions in terms of these variables.* The tri-

critical transition is an example where in general the scaling fields are not simply proportional to the experimental deviating fields. This has to be taken into account in the analysis of tricritical experiments.

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