Equations of State for Tricritical Points

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Renormalization-group recursion relations are used to calculate to order $\epsilon = 4-d$ the free-energy, ordering-susceptibility, and magnetization-crossover scaling functions for tricritical points in isotropic n-vector models. The equations of state describe critical and tricritical behavior in both ordered and disordered phases.

Much progress has resulted from the application of renormalization-group theory[1] to discuss ordinary critical points. In particular, these ideas have led to explicit calculations of critical exponents[1] and scaling functions[2] within the framework of the epsilon ($\epsilon = 4-d$) expansion. More complicated physical systems exhibiting multicritical behavior[3] have also been successfully analyzed. For example, critical exponents have been found characterizing tricritical systems,[4] as well as systems with spin-flop transitions.[5] However, little analytical progress has been made in calculating explicit crossover scaling functions describing multicritical behavior.[3] In this note, we report calculations to first order in $\epsilon = 4-d$ for a continuous classical spin model[4] of tricritical points.[6] The calculations give a description of the crossover from tricritical to lambda-line critical behavior. The tricritical exponents appearing in the theory are exact between three and four dimensions, while the critical-line exponents are correct to first order in ϵ. The theory accounts for the experimentally observed kink in the temperature-composition phase diagram for He^3-He^4 mixtures,[7] as well as in the analogous phase diagrams for the metamagnet $FeCl_2$.[8]

The method of calculation (which will be described briefly) allows scaling functions to be calculated directly from renormalization-group recursion relations. Riedel and Wegner[9] have applied a renormalization-group matching procedure to calculate the ordering susceptibility for certain somewhat *ad hoc* "recursion-relation models" of crossover behavior. We employ a similar approach here to calculate ordering-susceptibility, free-energy, and spontaneous-magnetization crossover scaling functions using exact recursion relations generated by the ϵ expansion. Such recursion relations exist for a variety of bicritical[5] and other multicritical crossover problems.[3] The procedure is more flexible than a conventional field-theoretic treatment,[10] and avoids the problems of exponentiating logarithms inherent in a direct Feynman graph approach.[2]

We consider the Landau-Ginzburg-Wilson Hamiltonian for isotropic n-component spins in d dimensions with S^6 interactions, namely,

$$\bar{\mathcal{H}} \equiv -\mathcal{H}/k_B T = \int dR\,[\tfrac{1}{2}(\nabla\vec{S})^2 + \tfrac{1}{2}r|\vec{S}|^2 + u|\vec{S}|^4 + v|\vec{S}|^6], \tag{1}$$

where

$$\vec{S} = \vec{S}(\vec{R}), \quad |\vec{S}|^2 = \sum_{i=1}^{n} S_i^{\,2}, \quad (\nabla\vec{S})^2 = \sum_{i,j=1}^{n,d} (\nabla_i S_j)^2,$$

and the components S_i vary between $\pm\infty$. We take v to be positive for thermodynamic stability. Riedel and Wegner[4] have argued heuristically that such a model could describe the tricritical point in ^{3}He-^{4}He mixtures. They proposed that the changeover from tricritical to lambda-line critical behavior corresponded to crossover Hamiltonian flows from a Gaussian to an n-component Heisenberg fixed point. This picture is borne out by explicit calculations near four dimensions,[1] and results in mean-field-theory tricritical exponents in three dimensions.[4] Here r and u are taken to be analytic functions of the chemical potential difference $\Delta = \mu_3 - \mu_4$ and the temperature T. Nelson and Fisher[11] have shown that a model for metamagnetic tricritical points can be collapsed into a Hamiltonian like (1), with r and u now functions of magnetic field and temperature. The Hamiltonian (1) has been treated in the spherical-model limit ($n \to \infty$) by Amit and De Dominicis,[12] and, more recently, by Emery.[13]

It is useful to present our results in the context of phenomenological crossover scaling theories,[14,15] supplemented by renormalization-group ideas.[4] The scaling description is expected to simplify when written in terms of appropriate linear combinations t, g, and w of the basic parameters r, u, and v appearing in (1).[4] In terms of these linear scaling fields, the singular part of tricritical free energy, for example, can be written near the tricritical fixed point (which is given by $t=g=w=0$ for $3\leqslant d\leqslant 4$) as

$$F(r,u,v)\approx t^{2-\alpha}\Phi(g/t^{\phi}, wt^{|\phi_v|}), \tag{2}$$

where α is the tricritical specific-heat index, and $\phi=\phi_u$ and $\phi_v=-|\phi_v|$ are crossover exponents. The conjecture of Riedel and Wegner,[4] that the Gaussian fixed point describes tricritical phenomena above three dimensions, leads to the formal scaling exponent predictions $\alpha=\frac{1}{2}\epsilon$, $\phi=\frac{1}{2}\epsilon$, and $|\phi_v|=1-\epsilon$. Although the exponents appearing in the formal scaling expression (2) are dimensionality dependent, singularities in $\Phi(x,y)$ when $d\geqslant 3$ cause many (but not all) "observed" tricritical indices to stick at their mean-field values as expected.[4] This phenomenon is related to the breakdown of hyperscaling above *four* dimensions (see Fisher,[16] and footnote 8 of Wegner and Riedel.[4] Usually one assumes[17] that the scaling function $\Phi(x,y)$ can be expanded in powers of $y=wt^{|\phi_v|}$, which becomes small as the tricritical point is approached, yielding

$$\Phi(x,y)\approx\Phi_0(x)+y(\partial\Phi/\partial y)_{y=0}+O(y^2), \tag{3}$$

with $\Phi_0(x)=\Phi(x,0)$. If the lambda-line singularities are to be described properly, $\Phi_0(x)$ should have a singularity at, say, $\mathring{x}$, as $x\to\mathring{x}^{\pm}$, of the form[15]

$$\Phi_0(x)\approx x^{(2-\alpha)/\phi}[A_\pm+B_\pm(x^{-1/\phi}-\mathring{x}^{-1/\phi})+C_\pm|x^{-1/\phi}-\mathring{x}^{-1/\phi}|^{2-\mathring{\alpha}}], \tag{4}$$

where $\mathring{\alpha}$ is the critical-line specific-heat index. This form differs slightly from that usually employed as it is designed to behave properly in the limit $\mathring{x}\to\infty$.[18] [The singularity in $\Phi_0(x)$ is indeed located at $\mathring{x}=\infty$ for tricritical points to $O(\epsilon)$; see Nicoll *et al.*[19] and below. If the critical hypersurface is to have a nonsingular shape, it is straightforward to show that $\mathring{x}$ should be strictly equal to inifinity.]

Our calculations are carried out to lowest order in $\epsilon=4-d$, assuming that r, u, and v are small. When u is positive, an expansion like (3) is possible, and the irrelevant variable v may be set equal to zero to obtain the leading behavior of the scaling functions. We find that the leading singular contribution to the free-energy density may be expressed in terms of the scaling field $t=r+(n+2)u/4\pi^2$ as

$$F(r,u,v)\approx[-nt^2/16u(4-n)][Q^{(4-n)/(n+8)}-1]+\min\{\tfrac{1}{2}t_RM^2+u_RM^4\}, \tag{5}$$

where

$$Q=Q(l^*)=1+(n+8)u(e^{\epsilon l^*}-1)2\pi^2\epsilon, \qquad t_R=tQ^{-(n+2)/(n+8)}, \quad u_R=uQ^{-1}, \tag{6}$$

and l^* is determined by the condition $|t_R|e^{2l^*}=1$. The quantity in braces must be minimized with respect to M, and the value $M=M_0$ thus obtained is the spontaneous magnetization. The ordering susceptibility is just the curvature about the minimum of the quantity in brackets. When (1) is viewed as a model for ^3He-^4He mixtures ($n=2$), the equation of the lambda line is $t=0$,[19] and the tricritical point is $(t,u)=(0,0)$. In the context of tricritical scaling,[7] $t=0$ denotes the scaling axis tangent to the tricritical point, while $u=0$ gives a second optimal scaling axis ($g=u$).

For fixed $\epsilon>0$ and small t and u, the results for the free energy, magnetization, and susceptibility may all be written in crossover scaling form. To see this, we note first that the equation determining l^* may be written as

$$te^{2l^*}=[1+(n+8)ue^{\epsilon l^*}/2\pi^2\epsilon]^{(n+2)/(n+8)} \tag{7}$$

near the tricritical point. Equation (7) defines a quantity $e^{l^*}=L(t,u)$ for every t and u. It is not hard to show that $L(t,u)$ satisfies a homogeneity relation, namely, $L(t,u)=bL(b^2t,b^\epsilon u)\equiv|t|^{-1/2}\phi(u/t^{\epsilon/2})$, with $\phi(x)=L(1,x)$. The behavior of $\phi(x)$ for small x (tricritical regime) and large x (critical regime) may be determined analytically from (7). When (7) is solved numerically for a given ϵ, it provides an interpolation between critical and tricritical behavior. To leading order, both the large-z and small-z behaviors are correctly given by $\phi(z)=[1+(n+8)z/2\pi^2\epsilon]^{(n+2)/2(n+8)}$. Various crossover scaling functions follow immediately; for example, the scaling function $\Phi_0(x)$ in the disordered phase for the free energy is

$$\Phi_0(x)=\frac{-n}{16(4-n)x}\left\{\left(\frac{1+(n+8)x[\phi(x)]^\epsilon}{2\pi^2\epsilon}\right)^{(4-n)/(n+8)}-1\right\}, \tag{8}$$

which has the behavior (4), with $\mathring{x}=\infty$, as $x\to\mathring{x}$. If we first set $\epsilon=0$, solving the equation $|t_R|e^{2l^*}=1$ produces a series of logarithmic corrections to critical behavior on the lambda line discussed by Larkin and Khmel'nitskii[20] and by Brézin.[21]

When u is negative, the full scaling function $\Phi(x,y)$ for the free energy (and other thermodynamic quantities as well) can no longer be expanded in its second argument, because a positive v is now necessary to stabilize the Hamiltonian (this is also true in a simple Landau theory). In this sense, v is analogous to the four-spin coupling constant above four dimensions (when $r<0$), which Fisher has called a "dangerous irrelevant variable."[16] We note, however, that a direct graphical analysis of (1) in three dimensions is possible far from the lambda line, the region amenable to such analysis including the first-order line.[22] The graphical analysis avoids approximations associated with an ϵ expansion and is thus complementary to our calculations with regard to the approach to the lambda line when u is positive. Nevertheless, a unified description of the scaling function associated with tricritical points remains an intriguing problem. By solving the appropriate renormalization-group recursion relations in an ϵ expansion, it is possible to construct a parabolic first-order surface[23] corresponding to a separating trajectory in Hamiltonian space. Analysis shows[23] that the temperature-composition phase diagram develops a kink at the tricritical point as $\epsilon\to 1$.[8,9] Emery[13] has produced this kink in the spherical-model limit ($n\to\infty$).

The basic result (5) for the free energy was derived directly from renormalization-group recursion relations. The basic principles involved are fairly simple. (A detailed account of our investigations, including a discussion of wave-vector–dependent susceptibilities and the effects of an ordering field, will be published elsewhere.[23]) We start by solving the differential recursion relations for r and u which, to $O(\epsilon)$, are[24]

$$\frac{dr}{dl}=2r+\frac{Au}{1+r},\quad \frac{du}{dl}=\epsilon u-\frac{Bu^2}{(1+r)^2},\tag{9}$$

where $A=(n+2)/2\pi^2$ and $B=(n+8)/2\pi^2$. The solutions to leading orders in ϵ and the coupling u are

$$r(l)=t(l)-\tfrac{1}{2}Au(l)+\tfrac{1}{2}Au(l)\,t(l)\ln[1+t(l)],\tag{10}$$

$$u(l)=u(0)e^{\epsilon l}/Q(l),\tag{11}$$

where

$$t(l)=t(0)e^{2l}/[Q(l)]^{(n+2)/(n+8)}\tag{12}$$

as may be verified by direct substitution into (9). These solutions are valid provided that r is not too large, so the integration of Eqs. (9) must be stopped at a value $l=l^*$ determined by $r(l^*)\approx 1$.

Although the results above are valid only in the disordered phase, a set of equations equivalent to (9) appropriate to the *ordered* phase can easily be derived by shifting the spin field in (1) by the exact magnetization. These equations have simple solutions expressible in terms of the functions $r(l)$ and $u(l)$ found in the *disordered* phase.[23] The integrations must now be stopped when $r(l^*)+12u(l^*)e^{(2-\epsilon)l^*}M_0^{\,2}$ is of order unity, where M_0 is the spontaneous magnetization.

Once the solutions of the recursion relations are known, the free energy in the critical regime can be related to a noncritical free energy far from T_c. With each renormalization-group iteration, a small spin-independent contribution to the free energy is generated,[25] and the free energy can be calculated by summing these contributions over many iterations.[25-28] The free energy then satisfies a modified homogeneity relation,[28] namely,

$$F(r,u)=\int_0^l G_0(l')e^{-l'd}\,dl' + e^{-ld}F(r(l),u(l)).\tag{13}$$

The first term can be thought of as a line integral along a renormalization-group trajectory, where the kernel $G_0(l)$ is just[26,28]

$$G_0(l)=(16\pi^2)^{-1}n\{\ln[1+r(l)]-\tfrac{1}{2}\}$$

to leading order. We evaluate (13) by choosing $l=l^*$ such that the correlation length associated with the "partially dressed" parameters $r(l^*)$ and $u(l^*)$ is of order unity, which corresponds to the limit of validity of our solutions to the recursion relations. Then, the free energy $F(r(l^*),u(l^*))$ can be calculated by a Landau theory with fluctuation corrections. Carrying out this program and extracting the leading behavior of the trajectory-integral term leads to our basic result (5). The prescriptions for obtaining the susceptibility and spontaneous magnetization follow because we have[1] $M_0=e^{-(1-1/2\epsilon)l}M_0(l)$, and $\chi=e^{2l}\chi(l)$, to $O(\epsilon)$, which can be used in the same way as Eq. (13).[9]

When u is negative, a full description of the tricritical behavior requires that (9) be replaced by three coupled differential equations[24] describing the evolution under iteration of r, u, and v.

The equation for the first-order line may be obtained by first integrating these equations until the correlation length is of order unity, and then applying the mean-field-theory criterion for a first-order transition to the partially dressed parameters.[23]

The techniques sketched above are quite general, and have proven useful in analyzing systems with cubic interactions[29] and anisotropic spin systems.[30]

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