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Renormalization-group results for the Blume-Capel model in two and three dimensions

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A Kadanoff lower-bound renormalization transformation with three variational parameters has been applied to the Blume-Capel model by Burkhardt. We report some additional results obtained in a particular one-parameter subspace of the three variational parameters. In this subspace the transformation treats the three possible Blume-Capel ground-state configurations with all the spins in the same state on an equal footing and preserves the three-state permutational symmetry of the Potts model. There are fixed points associated with first-order, critical, and tricritical transitions. The variational parameters maximizing the free energy at the critical and tricritical fixed points differ by only a few percent. The critical exponents associated with the different transitions and various points on the critical surfaces are calculated for $d = 2,3$ dimensions.

INTRODUCTION

The Blume-Emery-Griffiths-Potts model[1,2] has the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - K \sum_{\langle ij \rangle} \sigma_i^2 \sigma_j^2 + \Delta \sum_i \sigma_i^2 + H \sum_i \sigma_i , \quad (1)$$

where the spin variables σ take the values $\pm 1, 0$ and the exchange interactions only involve nearest neighbors. The Hamiltonian of the Blume-Capel model[3] is given by Eq. (1) with $K = 0$. The Hamiltonian of the three-state Potts model[4] is obtained from Eq. (1) by setting $J = \frac{1}{2} J_p$, $K = \frac{3}{2} J_p$, $\Delta = q J_p + \frac{1}{2}(\zeta_1 - 2\zeta_0 + \zeta_{-1})$, and $H = \frac{1}{2}(\zeta_1 - \zeta_{-1})$, where q is the coordination number of the lattice. The three-state Potts Hamiltonian is conventionally written in the equivalent form

$$\mathcal{H} = -J_p \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} + \sum_{i\alpha} \zeta_\alpha \delta_{\sigma_i \alpha} , \quad (2)$$

where the δ is a Kronecker delta and where α takes the values $\pm 1, 0$. If the fields ζ_α are all equal, the Potts model is invariant under permutations of the three spin states. In this paper we will be mainly concerned with the Blume-Capel model. For a global phase diagram in J, K, and Δ based on a position-space renormalization-group approach, we refer to an article by Berker and Wortis.[2]

Burkhardt[5] has analyzed the critical behavior of the Blume-Capel model using a Kadanoff lower-bound renormalization transformation[6] with three variational parameters $\vec{p}$. The calculation has two unsatisfactory aspects which are improved upon in this paper: (i) For $d = 2$ quite different variational parameters maximize the free energy at the critical and tricritical fixed points. For the optimum variational parameters of the critical fixed point there is no tricritical fixed point. To compute crossover behavior one must interpolate in $\vec{p}$. (ii) For $d = 3$ there appears to be no $\vec{p}$ maximizing the free energy at the tricritical fixed point.

In dealing with phase transitions which are not purely ferromagnetic, it is advisable to choose a renormalization transformation which treats the different ground states on an equal footing.[7] For the tricritical behavior of the Blume-Capel model the three possible ground-state configurations where all the spins are in the same state are of importance. For the case that all the site spins in a cell are the same, we impose the requirement that the weight function[6-8] relating the cell and site spins only take two possible values, W_+ if the cell spin equals the site spins and W_- otherwise. This condition restricts the three variational parameters of Ref. 5 to the one-parameter subspace $\vec{p} = p_0(1, -2, 3)$. Imposing the stronger condition that the renormalization transformation preserve the three-state permutational symmetry of the Potts model (with all the ζ_α equal) leads to the same one-parameter subspace.[9]

In the restricted subspace of variational parameters we have found discontinuity,[10] critical, and tricritical fixed points associated with first-order, second-order, and tricritical transitions in the Blume-Capel model and an anomalous tricritical point of the type discussed by Straley and Fisher[11] associated with the Potts transition (with all the ζ_α equal). The Potts tricritical results have been described by Dasgupta[12] and by Burkhardt, Knops, and den Nijs.[13] The optimum values of p_0 for the various critical and tricritical fixed points differ by only a few percent, and changing from one value to another causes no drastic changes in the fixed-

TABLE I. Critical and tricritical exponents. For $d=2$ $p_0^{(2)*}=0.7765$, $p_0^{(t)*}=0.8186$, $\vec{p}^{(2)*}=(0.7660,-\infty,\infty)$, $\vec{p}^{(t)*}=(2.983,-1.396,-0.07295)$. For $d=3$ $p_0^{(2)*}=0.4086$, $p_0^{(t)*}=0.4168$, $\vec{p}^{(2)*}=(0.4034,-\infty,\infty)$.

Critical exponents		$p_0^{(2)*}$	$\vec{p}^{(2)*}$	Known value or best estimate
$d=2$	$2-\alpha$	2.001	1.998	2
	δ	15.08	15.04	15
$d=3$	$2-\alpha$	1.887	1.887	1.92 ± 0.04
	δ	4.605	4.604	$5.0\ \pm0.2$
Tricritical exponents		$p_0^{(t)*}$	$\vec{p}^{(t)*}$	Known value or best estimate
$d=2$	$2-\alpha_t$	1.057	1.113	See Refs. 2, 5
	ϕ_t	0.4268	0.4445	
	δ_t	35.25	26.59	
$d=3$	$2-\alpha_t$	1.213	no $\vec{p}^{(t)*}$	$\frac{3}{2}$
	ϕ_t	0.2573	found	$\frac{1}{2}$
	δ_t	8.291		5

point topology. There is also an optimum value of p_0 for the $d=3$ ordinary tricritical point.

RESULTS

The values $p_0^{(2)*}$ and $p_0^{(t)*}$ which maximize the free energy at the critical and tricritical fixed points and the corresponding critical exponents are shown in Table I. For $d=2,3$ the ordinary critical exponents agree impressively with the known values and best estimates. The $d=2$ tricritical exponents may be compared with tables of Monte Carlo[14] and ϵ-expansion[15] results in Refs. 2 and 5. Our value of δ_t appears to be too large. The calculated $d=3$ tricritical exponents deviate considerably from the mean-field values predicted for $d\geq 3$ by Riedel and Wegner[16] using renormalization-group arguments. Surprisingly the $d=3$ Potts anomalous tricritical exponents[13] are much closer to those mean-field values.

Since the Blume-Capel model does not have the three-state permutational symmetry of the Potts model, one might expect improvement in the critical exponents upon leaving the subspace $\vec{p}=p_0(1,-2,3)$ in which the transformation preserves the permutational symmetry and optimizing with respect to all three variational parameters. This leads to $\vec{p}^{(2)*}$ and $\vec{p}^{(t)*}$ and the corresponding exponents in Table I. For the critical fixed points $p_2^{(2)*}\to-\infty$ and $p_3^{(2)*}\to\infty$ in such a way that the spin-1 renormalization transformation becomes equivalent to Kadanoff's spin-$\frac{1}{2}$ transformation[6] and yields identical critical exponents. The critical fixed points of Ref. 5 are different from the ones reported here (for $\vec{p}^{(2)*}$). Apparently the lower-bound transformation may yield more than one plausible candidate for a fixed point of a given type. The $d=2$ tricritical fixed point reported in Ref. 5 and here (for $\vec{p}^{(t)*}$) are the same. The $d=2$ $\vec{p}^{(t)*}$ tricritical exponents deviate from the Monte Carlo and ϵ-expansion results but are quite close to the values obtained in Ref. 2 with a different renormalization-group transformation. As in Ref. 5 no $\vec{p}^{(t)*}$ maximizing the free energy at the tricritical fixed point with respect to all three variational parameters could be found. From Table I one sees that maximizing with respect to all three variables does not substantially alter the critical exponents except in the case of δ_t, which depends very sensitively on its corresponding eigenvalue. The change in δ_t only represents a 1% change in the eigenvalue $y=\ln\lambda/\ln 2$.

One expects the discontinuity fixed point[10] associated with the line of first-order transitions (triple line) in the $H=0$ phase diagram to have two relevant operators with eigenvalue $y=d$, corresponding to the discontinuities in $\langle\sigma\rangle$ and $\langle\sigma^2\rangle$. With $p_0=p_0^{(2)*}$ both eigenvalues equal 1.984 for $d=2$ and 2.993 for $d=3$. As p_0 increases toward ∞, maximizing the fixed-point free energy, the fixed point moves toward ∞ in the space of coupling constants, and the relevant eigenvalues rapidly approach $y=d$.

Since $p_0^{(2)*}$ and $p_0^{(t)*}$ differ by only a few percent, the phase diagrams calculated with the two values are practically the same. Using an initial decimation transformation[5,6] followed by the lower bound transformation with $p_0^{(2)*}$, we find the $H=0$ phase diagram for the $d=2$ square lattice shown in Fig. 1. The intersection of the line of critical points with the $\Delta=0$ axis, which gives the critical temperature of the spin-1 Ising model, is at $J/k_BT=0.685$ (0.592) for the $d=2$ square lattice and at 0.241 (0.225) for the $d=3$ bcc lattice. The numbers in parentheses are series estimates.[17] For the Blume-Capel tricritical parameters we find Δ/qJ, k_BT/qJ to be 0.495, 0.133 for the $d=2$ square lattice and 0.472, 0.212 for the $d=3$ bcc lattice. Again the $d=2$ results are in better agreement with the quite different renormalization-group calculation of Ref. 2 than the Monte Carlo estimate[15] of 0.474 ± 0.003, 0.1925 ± 0.025 for a 100×100 lattice. The line of critical points and the first-order line intersect at the tricritical point with no interpolation in the variational parameters required. The first-order line intersects the $T=0$ axis at $\Delta/qJ=\frac{1}{2}$, in agreement with the exact result.

CLOSING REMARKS

That each fixed point has its own optimum variational parameters is a disadvantage of the lower

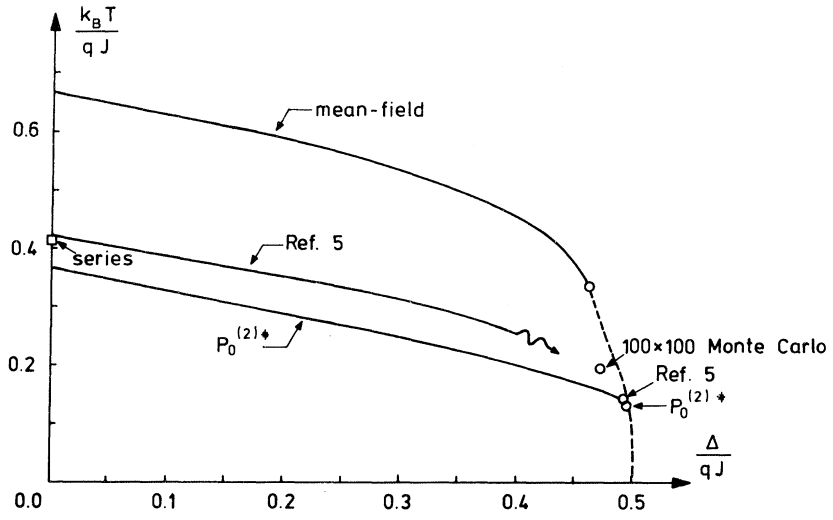

FIG. 1. Phase diagram for the $d=2$ square-lattice Blume-Capel model. The dashed and solid lines are lines of first- and second-order transitions, respectively. The circles indicate tricritical points. The phase diagram of Ref. 5 (only a portion of the second-order line is shown) was calculated with quite different variational parameters for the critical and tricritical fixed points. The lines of first- and second-order transitions do not intersect at the tricritical point. The phase diagram calculated with $p_0^{(2)*}$ has a less accurate second-order line but has the advantage that the entire phase diagram, with first- and second-order lines intersecting at the tricritical point, is obtained for a single choice of the variational parameters.

bound transformation as compared with the transformation of Ref. 2, especially when there are large numbers of fixed points. However the difficulty is not as serious as depicted in Ref. 5. In the restricted subspace of variational parameters the optimum p_0 for the critical, tricritical, and Potts-tricritical fixed points are roughly the same, and changing between the various values causes no drastic changes in the fixed-point topology.

As the three variational parameters in the lower-bound transformation are varied, complicated changes in the fixed-point topology involving large numbers of fixed points take place. It is useful to restrict the space of variational parameters to be investigated with physical considerations, as the results presented here demonstrate. Both the critical fixed points of Ref. 5 and this paper yield good values for the ordinary critical exponents. However the latter give a much more satisfactory description of tricritical crossover behavior since no interpolation in the variational parameters is required.

With the optimum $\vec{p}^{(2)*}$ for the critical fixed points of Ref. 5, the renormalization transformation has no tricritical and no discontinuity fixed points. But the critical fixed points of Ref. 5 give good values for the critical exponents and considerably better values (3% or 4% error) for the spin-1 Ising critical temperature than the critical fixed points of this paper. This is consistent with the observation that the $\vec{p}^{(2)*}$ of Ref. 5 weight configurations with cell spin ±1 more strongly than configurations with cell spin 0. Thus the transformation adequately describes Ising-like transitions, where there is little competition between the spin ±1 and spin-0 configurations, but fails in the tricritical and first-order regions.

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