Application of Kadanoff's lower-bound renormalization transformation to the Blume-Capel model

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The critical behavior of the Blume-Capel model for $d = 2,3$ is analyzed using a renormalization transformation based on Kadanoff's lower-bound transformation. There are fixed points associated with first-order, second-order, and tricritical phase transitions. The discontinuity fixed point onto which the line of first-order phase transitions is mapped has two relevant eigenoperators with eigenvalue 2^d, corresponding to the discontinuities in $\langle\sigma\rangle$ and $\langle\sigma^2\rangle$. Quite different values of the variational parameters in the renormalization transformation optimize the free energy at each fixed point, making it difficult to calculate crossover behavior with the present approach.

INTRODUCTION

The Blume-Capel model,[1] a special case of the Blume-Emery-Griffiths model,[2] has been widely discussed in connection with tricritical phenomena in magnetic systems and in ^{3}He-^{4}He mixtures. The spin-1 Hamiltonian with nearest-neighbor interactions has the form

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

where $\sigma_i = \pm 1, 0$. No exact solutions[3] of the model are available for $d \geq 2$, but Monte Carlo calculations for the $d = 2$ square lattice by Arora and Landau,[4] and exact series expansions for the $d = 3$ fcc lattice by Saul, Wortis, and Stauffer[5] confirm the gross features of the mean-field phase diagram[2] shown in Fig. 1. For $H = 0$ there is a tricritical point at the junction of a line of first-order and a line of second-order transitions. At $\Delta/qJ = \frac{1}{2}$ (q is the number of nearest neighbors), the first-order transition temperature goes to zero (an exact result). The tricritical exponents for $d = 3$ found in Ref. 5 are consistent with the mean-field exponents predicted for $d \geq 3$ by Riedel and Wegner[6] using renormalization-group (RG) arguments. Monte Carlo calculations[4] and ϵ expansions about $d = 3$ by Stephen and McCauley[7] and by Chang, Tuthill, and Stanley[8] give information about the $d = 2$ tricritical exponents.

In recent years block-spin RG transformations have been applied to the spin-$\frac{1}{2}$ Ising model with considerable success.[9-13] These transformations not only yield excellent values for the critical exponents but also permit one to calculate thermodynamic functions with surprising accuracy. This paper describes the application of a block-spin transformation similar to Kadanoff's spin-$\frac{1}{2}$ lower-bound transformation[12] to the Blume-Capel model.[14] Kadanoff's spin-$\frac{1}{2}$ transformation, which is based on a variational principle, has the advantages that it is quite simple, is not restricted to a particular dimension, and is extremely successful in predicting critical exponents. That the Blume-Capel model exhibits tricritical and first-order as well as second-order transitions makes it an especially interesting system to examine with block-spin RG methods.

The RG approach to phase transitions has largely been concerned with second- rather than first-order transitions. In calculations based on the ϵ expansion, the absence of a stable fixed point has been interpreted as evidence for a first-order transition.[15] Recently Nienhuis and Nauenberg[16] have introduced the concept of a discontinuity fixed point associated with first-order phase transitions and have analyzed tricritical and first-order transitions in a $d = 2$ spin-$\frac{1}{2}$ Ising metamagnet using a block-spin transformation.

Both the $d = 2$ and the $d = 3$ bcc lattices were considered in the calculations to be described. Before proceeding to a detailed discussion the main results will be briefly summarized.

For $d = 2$ one obtains a phase diagram (Fig. 1) with lines of first- and second-order transitions and a tricritical point, all in surprisingly good agreement with the Monte Carlo calculations of Ref. 4. The three types of transitions are associated with three different fixed points. The discontinuity fixed point onto which the first-order line is mapped has two relevant eigenoperators corresponding to the discontinuities in $\langle\sigma\rangle$ and $\langle\sigma^2\rangle$. Both eigenvalues equal the expected[16] value 2^d.

For $d = 2, 3$, the critical exponents of the line of second-order transitions (Table III) are in good agreement with known results and best estimates. The $d = 2$ tricritical exponents (Table IV) $2 - \alpha_t$ and ϕ_t are consistent with Monte Carlo results[4] and the ϵ expansion,[7,8] but δ_t is too large. For

$d=3$ there are no values of the three variational parameters $\vec{p}$ in the renormalization transformation which maximize the free energy of the tricritical fixed-point Hamiltonian within its domain of existence. In the domain the value of δ_t is considerably larger than the expected value, as in the case $d=2$.

The reason that the first- and second-order lines shown in Fig. 1 do not intersect is that they were calculated with different values of the variational parameters $\vec{p}$. Each fixed point has quite different optimal values of $\vec{p}$. If $\vec{p}$ is optimized for the tricritical fixed point, a distorted fixed-point topology near the second-order fixed point results, and vice-versa. In order to calculate crossover behavior, it is necessary to interpolate in $\vec{p}$. This is a practical difficulty with the present approach.

RENORMALIZATION TRANSFORMATION

The central ingredient in the RG approach is a transformation for converting a Hamiltonian with spin variables σ and interaction constants $\vec{K}$ into a Hamiltonian with new spin variables μ and new coupling constants $\vec{K}'$. The mapping increases the lattice constant of the system but leaves the partition function unchanged. In the present calculation, Hamiltonian operators are considered which may be written in the form $-\mathcal{H}/k_BT=\sum h$. In the case $d=2$, the sum extends over all squares of a square lattice, and h depends on $q=4$ spin variables. In the case $d=3$, the sum extends over all cubes of a simple-cubic lattice, and h depends on $q=8$ spin variables. The generalization of Kadanoff's spin-$\frac{1}{2}$ transformation[12] used in this paper has the form

$$h'(\mu_1\ldots\mu_q)=\ln \mathrm{Tr}_\sigma \exp[p_1(\mu_1\sigma_1+\cdots+\mu_q\sigma_q)+p_2(\mu_1^2+\cdots+\mu_q^2)+p_3(\mu_1^2\sigma_1^2+\cdots+\mu_q^2\sigma_q^2)+f(\sigma_1\cdots\sigma_q)+qh(\sigma_1\cdots\sigma_q)], \tag{2}$$

$$f(\sigma_1\ldots\sigma_q)=-\ln\{[2\cosh p_1(\sigma_1+\cdots+\sigma_q)]\exp[qp_2+p_3(\sigma_1^2+\cdots+\sigma_q^2)]+1\},$$

where μ and σ are spin-1 variables. The transformation yields a lower bound to the exact free energy. $\vec{p}=(p_1,p_2,p_3)$ are variational parameters adjusted to optimize the calculation.[17]

As discussed in Ref. 19, difficulties arising from an extra relevant variable are sometimes encountered if Kadanoff's transformation is used outside the invariant subspace of Hamiltonians in which $h(\sigma_1\cdots\sigma_q)$ is completely symmetric in the q-spin variables. To avoid such difficulties, an exact decimation transformation[11,12] is performed on the initial Hamiltonian to enter the symmetric subspace. In the $d=2$ square-lattice calculation the decimation eliminates every other spin, leaving a square lattice with a lattice constant increased by a factor $\sqrt{2}$. In the $d=3$ bcc calculation the decimation eliminates all of the spins on one of the two simple-cubic sublattices, leaving a simple-cubic lattice with the same lattice constant as the original bcc lattice. After the decimation is performed,

$$h(\sigma_1\cdots\sigma_q)=\ln\{2\cosh[(J/k_BT)(\sigma_1+\cdots+\sigma_q)]\times\exp(-\Delta/k_BT)+1\}-(q^{-1}\Delta/k_BT)(\sigma_1^2+\cdots+\sigma_q^2). \tag{3}$$

Here τ and σ represent the decimated and surviving spins, respectively.

With the substitution

$$h(\sigma_1\cdots\sigma_q)=\sum_\alpha K_\alpha S_\alpha(\sigma_1\cdots\sigma_q), \tag{4}$$

where the S_α are a complete set of spin operators symmetric in the q spin-1 variables, Eq. (2) may be reduced to a set of algebraic transformations involving the coupling constants

$$K'_\alpha=R_{\vec{p}}^{(\alpha)}(K_1,K_2,\ldots). \tag{5}$$

For $d=2$ there are nine operators with even-spin symmetry and six with odd-spin symmetry. They are shown in Table I. For $d=3$ there are 25 even and 20 odd operators. The fixed points $\vec{K}^*(\vec{p})$ of Eq. (5) determine the critical behavior of the system. The optimum value of $\vec{p}$ for a given fixed point is taken to be the value maximizing the free energy of the fixed-point Hamiltonian.[12,19]

RESULTS

The lower-bound transformation with initial decimation maps the lines of first- and second-order transitions and the tricritical point in the $H=0$ phase diagram onto three different fixed points. The second-order fixed point has one relevant eigenoperator with even spin symmetry, and the tricritical point has two.[6] The discontinuity fixed point[16,20] associated with the line of first-order transitions has one relevant eigenoperator with odd-spin symmetry and one with even symmetry, both with eigenvalue 2^d corresponding to the discontinuities in $\langle\sigma\rangle$ and $\langle\sigma^2\rangle$

For $d=2$ the three fixed points are listed in Table II. $\vec{p}^{(2)*}$ and $\vec{p}^{(t)*}$ maximize the free energy of the second-order and tricritical fixed-point

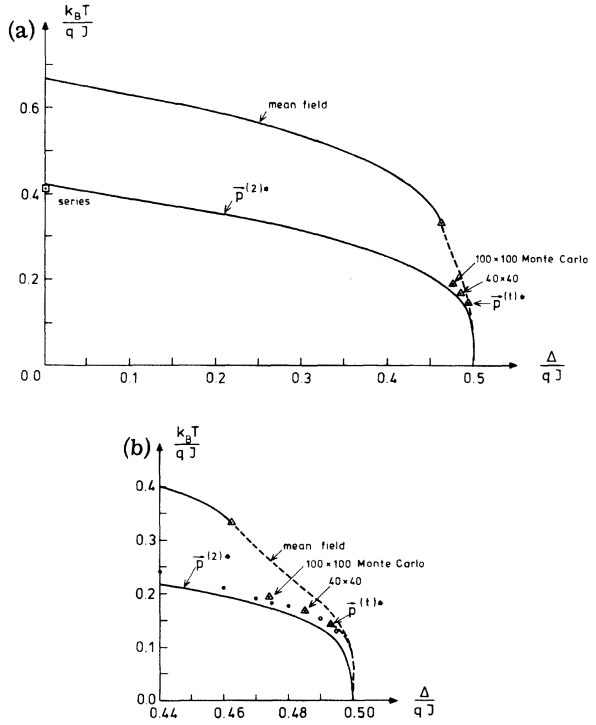

FIG. 1. Phase diagram for the $d=2$ square-lattice Blume-Capel model with zero magnetic field. The solid lines are lines of second-order transitions, and the dashed lines are lines of first-order transitions. The triangles denote tricritical points. The square labeled "series" denotes the value estimated from high-temperature series.[23,24] The upper curve shows the phase diagram obtained in mean-field theory.[2] $\vec{p}^{(2)*}$ denotes the line of second-order transitions obtained from the RG calculation with $\vec{p}=\vec{p}^{(2)*}$. $\vec{p}^{(t)*}$ denotes the tricritical point and the line of first-order transitions obtained from the RG calculations with $\vec{p}=\vec{p}^{(t)*}$. The solid and empty circles represent Monte Carlo results for the second- and first-order transitions, respectively, obtained for a 40×40 lattice (Ref. 4). The Monte Carlo tricritical points for both a 100×100 and a 40×40 lattice are shown.

Hamiltonians, respectively. The discontinuity fixed point is shown for $\vec{p}=\vec{p}^{(t)*}$. Its relevant even and odd eigenvalues are $\lambda_1^e=3.94$ and $\lambda_1^o=3.97$. As $\vec{p}$ moves toward the value maximizing the free energy of the discontinuity fixed-point Hamiltonian, the fixed point wanders towards infinity in the space of coupling constants, and the two relevant eigenvectors rapidly approach 2^d. As $\vec{p}$ passes through (2.673, −3.050, 0.5061), both eigenvalues equal 3.999 98. The next largest even and odd eigenvalues both have the value 0.047. A similar behavior is found for $d=3$, with both relevant eigenvalues approaching 8.

The tricritical entries for K_2^{e*} and K_3^{e*} in Table II indicate that the two-spin and crystal-field couplings are strong and opposing. The corresponding entries for the second-order transition are weak and cooperative. Because of the strong competing interactions one expects simple block-spin transformations to describe tricritical transitions less successfully than ordinary second-order transitions. This may be the origin of a problem encountered in the $d=3$ tricritical calculation. For $d=3$ there is no $\vec{p}^{(t)*}$ maximizing the free energy of the tricritical fixed-point Hamiltonian within its domain of existence in $\vec{p}$ space. For $d=3$, $\vec{p}^{(2)*}=(0.9026, -0.2711, -0.021\,89)$.

TABLE I. Nine operators with even-spin symmetry and the six operators with odd-spin symmetry considered in the $d=2$ calculation. Only the first term of each operator is shown. The others are obtained by symmetrizing the first term in the four-spin variables, if it is not already symmetric.

$S_1^e=1$	$S_1^o=\sigma_1+\cdots$
$S_2^e=\sigma_1\sigma_2+\cdots$	$S_2^o=\sigma_1\sigma_2\sigma_3+\cdots$
$S_3^e=\sigma_1^2+\cdots$	$S_3^o=\sigma_1^2\sigma_2+\cdots$
$S_4^e=\sigma_1\sigma_2\sigma_3\sigma_4$	$S_4^o=\sigma_1^2\sigma_2^2\sigma_3+\cdots$
$S_5^e=\sigma_1^2\sigma_2\sigma_3+\cdots$	$S_5^o=\sigma_1^2\sigma_2\sigma_3\sigma_4+\cdots$
$S_6^e=\sigma_1^2\sigma_2^2+\cdots$	$S_6^o=\sigma_1^2\sigma_2^2\sigma_3^2\sigma_4+\cdots$
$S_7^e=\sigma_1^2\sigma_2^2\sigma_3^2+\cdots$	
$S_8^e=\sigma_1^2\sigma_2^2\sigma_3\sigma_4+\cdots$	
$S_9^e=\sigma_1^2\sigma_2^2\sigma_3^2\sigma_4^2$	

Note that $\vec{p}^{(2)*}$ and $\vec{p}^{(t)*}$ in Table II are quite different. With the value $\vec{p}^{(2)*}$ in Eq. (5) there is no tricritical and no discontinuity fixed point. "Pair production" of the two fixed points occurs[21] at a value of p_2 more negative than $p_2^{(2)*}$. With the value $\vec{p}^{(t)*}$ in Eq. (5) there are spurious fixed points far from the tricritical and discontinuity fixed points. The optimum variational parameters depend rather sensitively on the particular fixed point in which one is interested. The parameters can be adjusted to give a locally but not a globally accurate picture of the fixed-point topology.

The calculated $d=2$ phase diagram is shown in Fig. 1. The RG lines of first- and second-order transitions do not intersect at the tricritical point since they were computed with $\vec{p}^{(t)*}$ and $\vec{p}^{(2)*}$, respectively. To compute lines which intersect, one needs to interpolate in $\vec{p}$. Each time the lower-bound transformation is applied, one should change $\vec{p}$ to a value appropriate to the changing location of the point in the space of Hamiltonians one is tracking.[22] This rather involved procedure represents a practical difficulty with the present approach. The intersection of the critical line in Fig. 1 with the k_BT/qJ axis, which gives the cri-

TABLE II. Fixed points associated with the second-order, tricritical, and first-order transitions for $d=2$. $\vec{p}^{(2)*}$ and $\vec{p}^{(t)*}$ maximize the free energy of the second-order and tricritical fixed-point Hamiltonians, respectively. $\vec{p}^{(2)*} = (1.095, -0.2165, -0.05118)$, $\vec{p}^{(t)*} = (2.983, -1.395, -0.07295)$.

	Second order, $\vec{p}^{(2)*}$	Tricritical, $\vec{p}^{(t)*}$	Discontinuity, $\vec{p}^{(t)*}$
K_2^{e*}	0.2313	0.3962	0.2818
K_3^{e*}	0.1488	−0.7423	−1.255
K_4^{e*}	−0.03595	−0.011 71	0.2614
K_5^{e*}	−0.03544	0.024 65	0.3325
K_6^{e*}	−0.026 28	0.085 28	0.1988
K_7^{e*}	0.015 16	−0.018 74	−0.029 32
K_8^{e*}	0.013 84	−0.005 926	−0.3003
K_9^{e*}	−0.011 90	−0.020 65	−0.1841

tical temperature of the spin-1 Ising model, is at $J/k_BT_c = 0.608$, as compared with the high-temperature series estimate[23,24] of 0.592. For $d=3$ the corresponding values[23] are 0.235 and 0.225. The coordinates of the RG tricritical point in Fig. 1, 0.493, 0.145 are in fair agreement with the Monte Carlo values[4] of 0.485, 0.169 for a 40×40 lattice, and 0.474 ± 0.003, 0.1925 ± 0.0025 for a 100×100 lattice. The RG line of first-order transition goes to $T=0$ at $\Delta/qJ=\frac{1}{2}$, as it should.

For the line of second-order transitions, the relevant eigenvalues and the critical exponents $2-\alpha = \ln 2^d/\ln\lambda_1^e$, and $\delta = \ln\lambda_1^o/\ln(2^d/\lambda_1^o)$ are shown in Table III. They agree impressively with the known values and best estimates.[12] An improvement in the calculated free energy does not guarantee improvement in the critical exponents. If p_2 and p_3 are set equal to zero in Eq. (2), the resulting one-parameter transformation naturally gives a poorer fit to the free energy. However, better values $2-\alpha = 2.009$ and $\delta = 15.34$ are obtained for the $d=2$ critical exponents, $p_1^{(2)*} = 0.9173$.

The $d=2$ tricritical exponents are compared with Monte Carlo results[4] and the ϵ expansion[7,8] in Table IV. The crossover[6] exponent ϕ_t was computed using $\phi_t = \ln\lambda_2^e/\ln\lambda_1^e$. $\beta_u = (1-\alpha_t)/\phi_t$. The most noticeable differences in the RG and Monte Carlo exponents are for δ_t, β_t, and β_u. The discrepancies in δ_t and β_t result from an 8% discrepancy in λ_1^o. Since α_t is nearly 1, the disagreement in β_u could stem from a much smaller relative discrepancy in α_t. The ϵ expansion should be interpreted cautiously because of the large ϵ^2 contribution to δ_t and the cancellation in β_t for $\epsilon=1$. To first order in ϵ with $\epsilon=1$, the ϵ expansion gives the sign of β_u incorrectly. As mentioned earlier, no $\vec{p}^{(t)*}$ apparently exists for $d=3$. However, everywhere I looked in the domain of existence of the tricritical point in $\vec{p}$-space, δ_t was larger than the expected value (the classical value $\delta_t=5$), as in the case $d=2$.

CONCLUDING REMARKS

In conclusion, I briefly compare the present approach with that of Nienhuis and Nauenberg, who have studied first-order, second-order, and tricritical transitions in a $d=2$ spin-$\frac{1}{2}$ Ising metamagnet using a block-spin transformation of the type introduced by Niemeyer and van Leeuwen[9]

TABLE III. Eigenvalues and critical exponents associated with the line of second-order transitions, computed for $\vec{p}=\vec{p}^{(2)*}$. There are two relevant eigenvectors with odd-spin symmetry. For $d=2$, $\lambda_1^e=1.958$, $\lambda_2^e=0.9791$, $\lambda_1^o=3.688$, $\lambda_2^o=1.125$; for $d=3$, $\lambda_1^e=3.011$, $\lambda_2^e=0.6500$, $\lambda_1^o=5.592$, $\lambda_2^o=1.500$.

Dimension	Exponent	This calculation	Exact value/best estimate (Ref. 12)
2	$2-\alpha=d\nu$	2.063	2
	δ	16.05	15
3	$2-\alpha=d\nu$	1.887	1.92 ± 0.04
	δ	4.805	5.0 ± 0.2

TABLE IV. Tricritical eigenvalues and exponents, computed for $\vec{p}=\vec{p}^{(t)*}$. There are two relevant eigenvectors with even-spin symmetry and two with odd-spin symmetry. $d=2$ and $\epsilon=3-d$. $\lambda_1^e=3.474$, $\lambda_2^e=1.739$; $\lambda_1^o=3.804$, $\lambda_2^o=2.153$.

Exponent	This calculation	Monte Carlo (Ref. 4)	ϵ expansion (Refs. 7 and 8)
$2-\alpha_t=d\nu_t$	1.113		$\frac{3}{2}-\frac{1}{2}\epsilon+\frac{3}{125}\epsilon^2=1.02$
δ_t	26.59	10.8 ± 0.7	$5+4\epsilon+\frac{997}{250}\epsilon^2=13.0$
ϕ_t	0.4445		$\frac{1}{2}+\frac{1}{10}\epsilon=0.6+O(\epsilon^2)$
β_t	0.040 36	0.09 ± 0.02	$\frac{1}{4}-\frac{1}{4}\epsilon+\frac{9}{2000}\epsilon^2=0.004\,50$
γ_t^-	1.033	1.0 ± 0.3	$1+\frac{3}{200}\epsilon^2=1.02$
γ_t^+	same	1.1 ± 0.4	same
β_u	0.2550	0.65 ± 0.10	$1-\frac{6}{5}\epsilon=-0.2+O(\epsilon^2)$

and refined by van Leeuwen.[25] Their transformation, which contains no adjustable parameters[26] and is set up for four cells of five spins each, exhibits all the fixed points associated with the different transitions.

Kadanoff's transformation has the advantage of extreme simplicity. Only 2^d spins are involved. The variational property permits the transformation to make the best of the small fundamental cluster, but the variational parameters must be appropriately adjusted for the particular region in the space of Hamiltonians in which one is interested. The adjustment produces a locally but not globally accurate picture of the fixed-point topology. To compute crossover behavior between distant fixed points, one must interpolate in the variational parameters. The transformation of Nienhuis and Nauenberg does not have this particular problem, but their transformation is very difficult to extend to $d=3$ or spin 1 for clusters large enough to give reliable quantitative results.

Note added in proof. H. J. F. Knops has pointed out to me that in the subspace of variational parameters $\vec{p}=p_0(1,-2,3)$, configurations with all spins 1, with all spins 0, and with all spins -1 are treated on an equal footing, which is desirable in considering tricritical behavior. Preliminary calculations for $d=2$ indicate the existence of critical, tricritical, and discontinuity fixed points in the subspace. The values of p_0^* for the critical and tricritical fixed points differ by only a few percent. On maximizing with respect to all three variational parameters, the critical exponents improve. The tricritical fixed point becomes equal to the one reported in this paper. The critical fixed point is different and becomes identical with Kadanoff's spin-$\frac{1}{2}$ fixed point. The details will be published.

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[21]Kadanoff's $d=2$ spin-$\frac{1}{2}$ lower-bound transformation also exhibits a tricritical and a discontinuity fixed point for p larger than 1.26. The tricritical parameters and the line of first-order transitions correspond to a four-spin coupling opposing the ferromagnetic two-spin coupling. There is no finite value of p maximizing the free energy of the tricritical fixed-point Hamiltonian.

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