Kadanoff's lower-bound renormalization transformation*

Theodore W. Burkhardt
Institut für Festkörperforschung der Kernforschungsanlage, D-517 Jülich, West Germany
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The fixed-point topology of Kadanoff's lower-bound renormalization transformation is discussed for the $d = 2$ square-lattice Ising model in the three-dimensional space of coupling constants for the nearest-neighbor, next-nearest neighbor, and four-spin interactions. An obstacle one encounters in trying to calculate a critical surface is pointed out. In the three-dimensional space of coupling constants Kadanoff's fixed point has two relevant vectors and can only be reached from a critical line, not from a critical surface. Another fixed point is reported which does have only one relevant vector and can be reached from a critical surface. The critical exponents of this fixed point are close to the exact values, though not nearly so close as for Kadanoff's fixed point. The properties of both fixed points as a function of the variational parameter p are described. Critical values of the nearest-neighbor couplings leading to the fixed points are compared.

I. INTRODUCTION

Kadanoff and co-workers[1,2] have recently calculated the critical behavior of the Ising and Wilson-Fisher models with a renormalization transformation[3,4] based on a lower-bound variational approximation to the free energy. The transformation is quite simple and is not restricted to a particular dimension. The Ising critical exponents for $d=2$, 3, 4 agree very impressively with known results. Thermodynamic functions for the $d=2$ Ising model closely approximate the exact Onsager solution.

In applying the lower-bound renormalization transformation (LBRT) to the $d=2$ square-lattice Ising model without external field, Kadanoff and co-workers parametrize the nearest-neighbor, next-nearest neighbor, and four-spin interactions in the sequence of Hamiltonians with coupling constants[5] $K_{\rm nn}$, $K_{\rm nnn}$, and K_4. They perform their calculations in an invariant subspace of the LBRT in which $K_{\rm nn}=K_{\rm nnn}$. In considering an initial Hamiltonian which only contains nearest-neighbor interactions, they first perform a decimation transformation[6] (an exact procedure) to enter the subspace $K_{\rm nn}=K_{\rm nnn}$ before repeatedly applying the LBRT.

U sing a different recursion formula based on a cluster-approximation method developed by Niemeijer and Van Leeuwen,[7] Nauenberg and Nienhuis[8] have also calculated the thermodynamic functions of the $d=2$ square-lattice Ising model. They obtained a surprisingly accurate picture of the critical surface in the variables $K_{\rm nn}$, $K_{\rm nnn}$, and K_4. One advantage of Kadanoff's LBRT is that it can be more readily extended to higher dimensions than the cluster-approximation method. An interesting question is whether the LBRT can also be used to furnish an accurate picture of the critical surface of the Ising model.

In this paper the fixed-point topology of the LBRT for the $d=2$ square-lattice Ising model is discussed in the three-dimensional space of variables $K_{\rm nn}$, $K_{\rm nnn}$, and K_4 not just in the subspace $K_{\rm nn}=K_{\rm nnn}$. An obstacle one encounters in trying to calculate a critical surface for the Ising model is pointed out. In addition to a relevant and an irrelevant eigenvector[3,4] in the subspace $K_{\rm nn}=K_{\rm nnn}$, Kadanoff's fixed point has an eigenvector outside the subspace, which goes from irrelevant to relevant as the variational parameter p passes through the value $p_b=0.741$. For the optimum value $p^*=0.766$ used in calculating critical exponents the fixed point can only be reached from a critical line in the $K_{\rm nn}=K_{\rm nnn}$ subspace, not from all points on a critical surface as one would expect. A second critical point, which lies outside the $K_{\rm nn}=K_{\rm nnn}$ subspace and has only one relevant vector, is reported. This fixed point, which originates at $p=p_b$ in a bifurcation occurring at Kadanoff's fixed point, only exists for $p>p_b$. Its critical exponents $2-\alpha$ and δ are 1.966 and 15.36 as compared with 1.998 and 15.04 for Kadanoff's fixed point, and 2 and 15 for the exact exponents. The critical exponents of both fixed points are described as a function of p. Critical values of the nearest-neighbor coupling calculated for the two fixed points are compared, with Kadanoff's procedure, a decimation followed by the LBRT, giving somewhat better results.

In the Sec. II the explicit form of the LBRT for the $d=2$ Ising model is briefly reviewed. In Sec. III the new results referred to above are described.

II. LOWER-BOUND RENORMALIZATION TRANSFORMATION

In applying the LBRT to the $d=2$ square-lattice Ising model without external field,[1,2] one considers a sequence of Hamiltonian with the form

$$H_{\vec{K}}(\sigma) = -\sum_{\text{squares}} \sum_{i} K_i s_i(\sigma) \ . \tag{1}$$

The sum over i includes the four spin operators

TABLE I. Four spin operators in the sequence of Hamiltonians and the four independent classes of spin configurations. n_i gives the number of distinct spin configurations in class i.

i	s_i	Configurations	n_i
0	$s_0 = 1$	$++++, ----$	2
nn	$s_{nn} = \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1$	$+++-, ---+$, cyclic permutations	8
nnn	$s_{nnn} = \sigma_1\sigma_3 + \sigma_2\sigma_4$	$++--$, cyclic permutations	4
4	$s_4 = \sigma_1\sigma_2\sigma_3\sigma_4$	$+-+-, -+-+$	2

shown in Table I. They form a complete set of even operators reflecting the point-group symmetry of a square of four spins. The LBRT generates an $H'_{\vec{K}'}(\mu)$ from $H_{\vec{K}}(\sigma)$. The μ variables are Ising spins on a lattice with twice the lattice constant of the σ lattice. The transformation has the explicit form

$$\exp\Big(\sum_i K'_i s_i(\mu)\Big) = \mathrm{Tr}_{\sigma_1\cdots\sigma_4} \exp\Big(p(\mu_1\sigma_1 + \cdots \mu_4\sigma_4) - \ln 2\cosh p(\sigma_1 + \cdots \sigma_4) + 4\sum_i K_i s_i(\sigma)\Big) , \quad (2)$$

where p is a variational parameter adjusted to maximize the free energy.

To obtain algebraic equations relating the K'_i's and K_i's, one chooses particular configurations for the μ spins in Eq. (2). Each of the four classes of configurations in Table I yields an independent equation. The algebraic structure becomes especially clear if new variables $z_i = \exp(\sum_j X_{ij}K_j)$ are introduced. The matrix $X_{ij} = s_j|_{\text{config. } i}$ is given in Table II. In terms of z_i the LBRT has the form

$$z'_i = \sum_j w_{ij} z_j^4 , \quad (3)$$

where

$$w_{ij} = (1/n_i)\,\mathrm{Tr}_{\substack{\sigma_1\cdots\sigma_4 \\ \mu_1\cdots\mu_4}} \{P_i(\mu)P_j(\sigma)\exp[p(\mu_1\sigma_1 + \cdots \mu_4\sigma_4) - \ln 2\cosh p(\sigma_1 + \cdots \sigma_4)]\} . \quad (4)$$

Here P_i is a projection operator onto class i of the four classes of spin configurations in Table I. n_i, the number of distinct spin configurations in class i, is listed in Table I. When the trace in Eq. (4) is evaluated, the expression for w shown in Table II is obtained.

The fixed points of the LBRT satisfy the nonlinear equation

$$z_i^* = \sum_j w_{ij} z_j^{*4} . \quad (5)$$

The right eigenvectors δz_i and eigenvalues λ associated with the fixed point are solutions of the linear equations[9]

$$4\sum_j w_{ij} z_j^{*3} \delta z_j = \lambda \delta z_i . \quad (6)$$

That the symmetry $K_{nn} = K_{nnn}$ is preserved by the LBRT may readily be seen from Eq. (2). If $K_{nn} = K_{nnn}$, the exponential factor on the right-hand side is completely symmetric under interchange of any two σ spins. This implies that the left-hand side is completely symmetric under interchange of any two μ spins. Consequently $K'_{nn} = K'_{nnn}$. The subspace $K_{nn} = K_{nnn}$ corresponds to the subspace $z_3 = z_4$ in the variables z_i (replacing the indices $i = 0$, nn, nnn, 4 with $i = 1, 2, 3, 4$). From Eq. (3) and the explicit form of w in Table II it can immediately be verified that $z'_3 = z'_4$ if $z_3 = z_4$.

An additional property of the LBRT will be used in Sec. III. For any fixed point in the subspace $z_3 = z_4$, one solution of Eq. (6) is

$$\delta\vec{z} = (0, 0, 1, -2) , \quad \lambda = 8z_3^{*3}(\cosh^2 p - 1) . \quad (7)$$

This eigenvector lies outside the invariant subspace, and its direction is independent of the variational parameter p. In the space of the variables K_i the eigenvector has the direction

$$\delta\vec{K} = (0, 1, -2, 0) . \quad (8)$$

As discussed in Refs. 1 and 2, for an initial Hamiltonian with coupling constants $\vec{K}^{(0)}$, a lower bound to the free energy per particle $f_p(\vec{K}^{(0)})$ may be computed from the limit

$$f_p(\vec{K}^{(0)}) = -\lim_{\alpha\to\infty} \frac{K_0^{(\alpha)}}{4^\alpha} , \quad (9)$$

TABLE II. Matrices X and w.

$$X = 8X^{-1} = \begin{pmatrix} 1 & 4 & 2 & 1 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & -2 & 1 \\ 1 & -4 & 2 & 1 \end{pmatrix}$$

$$w = \begin{pmatrix} 1 & 4 & 2 & 1 \\ \frac{q}{2q^2-1} & \frac{2}{q}(q^2+1) & 2q & q \\ \frac{1}{2q^2-1} & 4 & 2q^2 & 1 \\ \frac{1}{2q^2-1} & 4 & 2 & 2q^2-1 \end{pmatrix}$$

where $q = \cosh p$

TABLE III. Five fixed points of the LBRT, their eigenvalues with even spin symmetry, and their eigenvectors, computed for $p = 0.76$.

Fixed point	K_{nn}^*	K_{nnn}^*	K_4^*	λ^e	δK_{nn}	δK_{nnn}	δK_4
(1s)	−0.1621	−0.1621	0.08366	2.908	1	−2	0
				0.2243	1	1	−0.9115
				0.005114	1	1	1.009
(2s)	0.2754	0.2754	−0.1266	0.3048	1	1	−0.9590
				0.03447	1	1	−3.255
				0.05033	1	−2	0
(3s)	0.1400	0.1400	−0.008825	1.970	1	1	−0.6201
				1.113	1	−2	0
				0.4903	1	1	−6.306
(1)	−0.0005864	−0.4225	0.0003959	0.1111	1	−11.00	−0.6890
				0.01816	1	−0.7319	−0.8032
				0.001750	1	1.021	1.028
(3)	0.1578	0.1092	−0.007943	2.015	1	1.738	−0.7998
				0.8920	1	−1.589	0.1695
				0.4497	1	−0.5086	−2.776

where $K_0^{(\alpha)}$ is the value of K_0 after α applications of the LBRT. For the optimum value of p, $g_p(\vec{K}^{(0)}) = 0$ where

$$f_{p+\Delta p}(\vec{K}^{(0)}) - f_p(\vec{K}^{(0)}) = g_p(\vec{K}^{(0)})\Delta p + O((\Delta p)^2) . \quad (10)$$

In calculating critical exponents, Kadanoff and co-workers maximize the free energy for an initial Hamiltonian equal to the fixed-point Hamiltonian. They choose the $p = p^*$ and $\vec{K}^*(p)$ for which $g_{p^*}(\vec{K}^*(p^*)) = 0$.

III. RESULTS

Table III lists five fixed points[10] of the LBRT and their eigenvectors and eigenvalues, computed for $p = 0.76$. As will be explained below in more detail, (1s) and (1) are high-temperature fixed points, (2s) is a low-temperature fixed point, and (3s) and (3) are critical fixed points. The subscript s indicates a fixed point in the subspace $K_{nn} = K_{nnn}$.

For both fixed points (3s) and (3) the values of the critical exponents $2 - \alpha$ and δ computed from the largest nontrivial eigenvalues with even and odd spin symmetry are close to the exact Onsager values. When p is optimized according to the prescription following Eq. (10), the results shown in Table IV are obtained. Fixed point (3s) was reported by Kadanoff and co-workers. It has a relevant ($\lambda > 1$) and an irrelevant ($\lambda < 1$) eigenvector in the subspace $K_{nn} = K_{nnn}$ and an additional relevant eigenvector outside the subspace, which is the eigenvector shown as Eq. (8). Thus (3s) can only be approached along a critical line in the $K_{nn} = K_{nnn}$ subspace. Fixed point (3) has only one relevant vector, as one would expect for the Ising critical fixed point, and can be approached from a critical surface. However its critical exponents are not so close to the exact exponents as those of Kadanoff's fixed point.

In considering an initial Hamiltonian containing only nearest-neighbor interactions, Kadanoff and co-workers first perform a decimation transformation to reach the subspace $K_{nn} = K_{nnn}$. This transformation, which is exact if the initial Hamiltonian only contains nearest-neighbor interactions, eliminates every other spin, increasing the lattice constant by the factor $\sqrt{2}$. It has the form

$$\begin{aligned} K_0' &= \tfrac{1}{8}\ln\cosh 8K_{nn} + \tfrac{1}{2}\ln\cosh 4K_{nn} + \ln 2 , \\ K_{nn}' &= K_{nnn}' = \tfrac{1}{8}\ln\cosh 8K_{nn} , \\ K_4' &= \tfrac{1}{8}\ln\cosh 8K_{nn} - \tfrac{1}{2}\ln\cosh 4K_{nn} . \end{aligned} \quad (11)$$

TABLE IV. Critical exponents and values of the critical nearest-neighbor coupling. p^* is the value of p which maximizes the free energy for an initial Hamiltonian equal to the fixed point Hamiltonian. $p^\dagger$ maximizes the free energy for an initial Hamiltonian containing only the critical nearest-neighbor coupling.

Fixed point	p^*	$2-\alpha$	δ
(3s)	0.7660	1.998	15.04
(3)	0.7610	1.966	15.36
Exact exponents		2	15
Decimation followed		$p^* = 0.766$	$K_{nn}^c = 0.229$
by LBRT		$p^\dagger = 0.773$	$K_{nn}^c = 0.229$
LBRT without		$p^* = 0.761$	$K_{nn}^c = 0.242$
initial decimation		$p^\dagger = 0.730$	$K_{nn}^c = 0.239$
Exact value		$K_{nn}^c = \frac{1}{4}\ln(1+\sqrt{2}) = 0.220$	

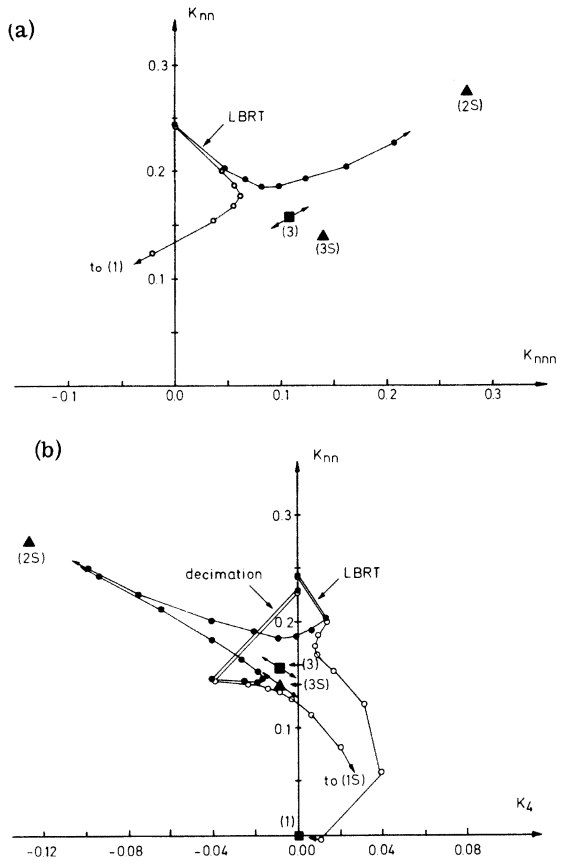

FIG. 1. Trajectories generated by the LBRT with and without an initial decimation from an initial Hamiltonian only containing nearest-neighbor interactions. The projections of the trajectories onto the planes $K_4 = 0$ and $K_{nnn} = 0$ are shown. For the dark and light circles $K_{nn}^{in} = K_{nn}^{c} \pm 0.001$, respectively. The arrows through the fixed points denote the directions of relevant eigenvectors. The exact value of K_{nn}^{c} is 0.220.

After the decimation transformation they repeatedly apply the LBRT. Following this procedure one finds (see Fig. 1) a critical value K_{nn}^{c} of the initial nearest-neighbor coupling constant K_{nn}^{in} with the following properties: For $0 < K_{nn}^{in} < K_{nn}^{c}$ the trajectory goes to fixed point (1s) (high-temperature fixed point), and for $K_{nn}^{in} > K_{nn}^{c}$ the trajectory goes to (2s) (low-temperature fixed point). If K_{nn}^{in} is sufficiently close to K_{nn}^{c}, the trajectory approaches (3s) arbitrarily closely before veering off to (1s) or (2s). The initial decimation transformation is absolutely essential for reaching (3s) since the critical line along which (3s) can be approached lies in the $K_{nn} = K_{nnn}$ subspace.

If the LBRT is repeatedly applied to a starting Hamiltonian containing only nearest-neighbor interactions without first performing a decimation, one finds (see Fig. 1) that for $0 < K_{nn}^{in} < K_{nn}^{c}$ the trajectories always go to (1) and for $K_{nn}^{in} > K_{nn}^{c}$ to (2s).

When K_{nn}^{in} is sufficiently close to K_{nn}^{c}, the trajectory approaches (3) arbitrarily closely. There is no value of K_{nn}^{in} for which the trajectory goes to (3s).

The position of fixed point (3s) in the space of coupling constants is a slowly varying function of p. In this respect (3) is strikingly different. Below the value $p = p_b = 0.741$ (3) does not exist at all. (3s) is the only critical fixed point, and the eigenvector shown as Eq. (8) is irrelevant, so that (3s) has the topology expected for the exact Ising fixed point. At $p = p_b$ the eigenvector becomes marginal ($\lambda = 1$), and bifurcation occurs at (3s). As p is further increased, the marginal eigenvector becomes relevant, and (3) moves away from (3s) in the direction of the new relevant vector.

The largest nontrivial eigenvalue with even spin symmetry λ_1^e, the next largest λ_2^e (the eigenvalue which is marginal at p_b), and the largest eigenvalue with odd spin symmetry λ_1^o, are shown as a function of p for both critical fixed points in Fig. 2. The critical exponents $2 - \alpha$ and δ are related to λ_1^e and λ_1^o, by the formulas

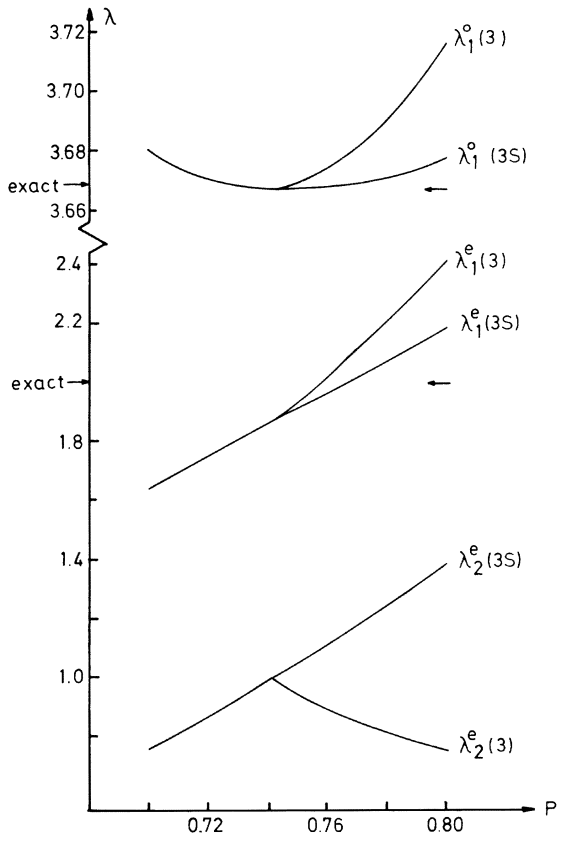

FIG. 2. Largest nontrivial eigenvalue with even spin symmetry λ_1^e, the next largest λ_2^e, and the largest eigenvalue with odd spin symmetry λ_1^o, of fixed points (3s) and (3) as a function of p. (3) exists only for $p > p_b = 0.741$. At $p = p_b$, $\lambda_2^e = 1$. The arrows on the λ axis marked "exact" denote the Onsager values for λ_1^e and λ_1^o.

$$2-\alpha=\ln 4/\ln\lambda_1^e\ ,$$
$$\delta=\ln\lambda_1^o/\ln(4/\lambda_1^o)\ . \qquad (12)$$

Some results for the critical value of the nearest-neighbor coupling are shown in Table IV. Two methods of choosing the optimum value of p were considered. One method, already discussed, is to use the p which maximizes the free energy of the fixed-point Hamiltonian, i.e., $g_{p^*}(\vec{K}^*(p^*))=0$. The second method is to use the value $p^\dagger$ which maximizes the free energy of the starting Hamiltonian containing only the critical nearest-neighbor coupling constant, i.e., $g_{p^\dagger}(K_{nn}^c(p^\dagger))=0$. The procedure of Refs. 1 and 2, a decimation followed by the LBRT, gives the best results. If the LBRT is used without an initial decimation, $p^\dagger=0.730$. Since $p^\dagger<p_b=0.741$, for $p=p^\dagger$ $(3s)$ is the only critical fixed point and has only one relevant vector in K_{nn}, K_{nnn}, and K_4 space.

IV. CONCLUSIONS

The difficulty one encounters in trying to calculate a critical surface with the LBRT may be summarized as follows: Kadanoff's fixed point, which yields critical exponents for $d=2$, 3, 4 amazingly close to the exact values, can only be approached from a critical line in the subspace $K_{nn}=K_{nnn}$. To calculate a critical surface for the fixed point, an initial transformation must be performed to enter the subspace. For an initial Hamiltonian containing nearest-neighbor interactions only, an exact decimation transformation is available, but for arbitrary values of the initial coupling constants a different transformation is needed. There is another fixed point outside the subspace $K_{nn}=K_{nnn}$ which can be reached from a critical surface via the LBRT, but its critical exponents are not nearly so close to the exact values as those of Kadanoff's fixed point.

It should be emphasized that the calculation of a realistic critical surface is quite a severe test for an approximate recursion relation. The standard critical exponents are solely determined by the largest nontrivial eigenvalues with even and odd spin symmetry of the transformation linearized at the fixed point. Additional information must be accurately produced to furnish a faithful picture of the critical surface as well. In an approximation in which an infinite set of coupling constants is replaced by three, it is not surprising that some features of the exact solution are lost.

The difficulty one encounters in trying to calculate a critical surface with the LBRT is closely connected with the special role of the symmetric subspace $K_{nn}=K_{nnn}$ in the transformation. A desirable goal in improving the LBRT would be to eliminate this special role in as far as it is an unphysical artifact of the approximation and to incorporate those exact symmetries of the Ising free energy (such as invariance under $K_{nn}\to -K_{nn}$) which are not preserved by the LBRT in its simplest form.

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[5]The coupling constants are defined by Eq. (1) and Table I. K_{nn} is $\frac{1}{2}$ the conventionally-defined nearest-neighbor coupling, whereas K_{nnn} is the same as the conventionally-defined quantity.

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[9]From the form of w in Eq. (4) it is straightforward to prove that the eigenvalues λ are real and positive, as was pointed out to me by Dr. David Wallace.

[10]For $p=0.76$ there is at least one other stable fixed point (which trajectories generated from an initial Hamiltonian containing only nearest-neighbor couplings with $K_{nn}<0$ approach). For larger values of p at least two additional unstable fixed points exist.