JOURNAL OF COMPUTATIONAL PHYSICS 43, 289–314 (1981)

Direct Calculation of the Derivatives of the Free Energy for Ising Models by a Modified Kadanoff Variational Method*

CHIN-KUN HU AND P. KLEBAN

Department of Physics and Astronomy, and Laboratory for Surface Science and Technology, University of Maine, Orono, Maine 04469

Received February 3, 1981; revised June 26, 1981

A systematic procedure is presented for the direct calculation of the free energy and its first and second derivatives with respect to temperature or external field for Ising models in one to three dimensions with a wide class of interactions. These are classified by their point group symmetry properties. This renormalization group method is based on the modified Kadanoff variational method (MKVM). This method is not only general, but also very accurate numerically both near and far from the critical point. Further, it includes correction to scaling effects not present in the standard linearized renormalization group treatment. This work describes the technique and presents some illustrative results for the square lattice and body-centered cubic lattice with nearest neighbor interactions.

I. INTRODUCTION

In recent years, the position space renormalization group (PSRG) method and its application to phase transitions of various spin models has been widely studied. One important example is Kadanoff's lower bound renormalization group transformation (LBRGT) [1].

In Kadanoff's LBRGT, one has variational parameters in the renormalization group transformation (RGT) equation relating transformed and original unit cell potentials. The optimum variational parameters must be chosen in order to get the best lower bound free energy from the transformed Hamiltonian. Several different methods with different degrees of complexity [2–4] have been proposed to determine these variational parameters. One such method is the Modified Kadanoff Variational Method (MKVM) [3].

In the MKVM, the variational parameter p is determined by minimizing the single cell free energy. This leads to an analytic nonlinear equation for p. In previous work [3, 5], it was found that the MKVM is very accurate for two-valued spin models without external magnetic field, in one or two dimensions. It has also been applied to the three-dimensional Ising model on a BCC lattice, where the derivatives of the free energy were calculated by numerical differentiation of the free energy [6]. In three

* Work supported by the Office of Naval Research.

0021-9991/81/100289-25$02.00/0

581/43/2-7

dimensions the critical temperature obtained is within 3% of the series expansion value [12].

In this paper, we formulate a systematic procedure for directly calculating the free energy and its first and second derivatives with respect to temperature and external magnetic fields for a wide class of Ising models based on the MKVM. In this way we avoid the errors arising from numerical differentiation, and thus have more accurate derivatives of the free energy. These quantities, including specific heat, spontaneous magnetization and magnetic susceptibility, are the physically interesting quantities in most cases.

In the application of RG theory to phase transitions, one usually formulates the RGT equations for the coupling constants, then solves them for the fixed point solution(s) and finally expands the RGT equations around the fixed points to find the linearized RGT equations and their eigenvalues and hence critical exponents. In this work we take a slightly different approach. Here we apply the RGT to the Hamiltonian of the given system and calculate the free energy and its first and second derivatives directly. We determine the critical temperature of the given system in the standard way, by examining the behavior of the variational parameters and coupling constants (which tend to larger or smaller values, when one is at temperatures below or above this critical point, respectively). Then, by analyzing the values of the first and second derivatives of the free energy near the critical point, we can determine critical exponents, critical amplitudes and other critical parameters including their less divergent corrections which are of considerable current interest [7, 8]. This analysis, which resembles the extraction of critical parameters from experimental data, is very involved and will be presented elsewhere. A preliminary least squares analysis for the Ising model on the BCC lattice indicates that $\alpha > \alpha'$, i.e., the specific heat appears to diverge less strongly when the critical temperature is approached from below. (This can occur because we are determining effective critical exponents—if one approaches the critical point sufficiently closely, our results reduce to those of the standard linearized RGT.)

Since the quantities of direct interest here are free energies and their derivatives, instead of the fixed point and linearized RGT, it is not necessary to carry out the calculation in coupling constant space. In fact, to write a single computer program applicable to many systems with different symmetry properties, it is more convenient to carry out the calculation in cell potential space. This is related to coupling constant space by a linear transformation.

The present paper is organized as follows: In Section II, we derive formulas for free energies and their first and second derivatives with respect to temperature and external magnetic field. These formulas are written in cell potential space instead of coupling constant space. In Section III, we consider some typical systems with various symmetry properties in one to three space dimensions. We show that we may use very simple criteria to classify all possible spin configurations on a unit cell into different degeneracy groups, each of which corresponds to an independent cell potential. The systems considered are listed in Table I.

We illustrate our formalism in Section IV by calculating the free energy and its

first and second derivatives with respect to temperature and external magnetic field for Ising models on two-dimensional square and three-dimensional BCC lattices. Our results are compared with exact [9, 10] and series expansion values [11, 12] and are shown in Figs. 1 and 2. It is clear from the figures that our method gives very accurate values for derivatives of the free energy over a wide range of temperatures away from the critical point. When one is very close to the critical point, our results reduce to those of the standard linearized RG treatment. However, as pointed out above, our method also includes the possibility of less divergent corrections to critical behavior when one is near the critical point. A full analysis of this behavior is a non-trivial task and will be described elsewhere.

II. General Formalism

Let us consider N Ising spins σ_i $(= \pm 1)$ on a general d dimensional lattice, which interact with each other via a Hamiltonian of the form [1]:

$$\beta H(\sigma_1, \sigma_2, ..., \sigma_N) = -\sum_{R'} v_{R'}(\sigma_{R'}), \tag{1}$$

where $\sum_{R'}$ is a sum over all d dimensional hypercube unit cells of the lattice. Note that these cells differ from the usual renormalization group cells in that here a given spin may be in more than one cell. $\sigma_{R'} = \{\sigma_1, ..., \sigma_z\}$ with $z = 2^d$ are spins at the corners of the unit cell R' and $v_{R'}(\sigma_{R'})$ is the interaction potential of the spins $\sigma_{R'}$ within the unit cell R'. After a Kadanoff LBRGT, the transformed Hamiltonian for N' Ising spins $\mu_i(=\pm 1)$ on lattice with double lattice spacing has the same form as that of Eq. (1), i.e.,

$$\beta' H'(\mu_1, \mu_2, ..., \mu_{N'}) = -\sum_{R} v'_R(\mu_R), \tag{2}$$

where N' is the number of spins on the new lattice $(N' = N/z)$, v'_R (μ_R) is the interaction potential for the Ising spins $\mu_R = \{\mu_1, ..., \mu_z\}$ on a hypercube unit cell R with double the original lattice spacing, and v'_R is related to $v_{R'}(\sigma_{R'})$ by the RGT equation (hereafter we will drop the subscripts on $v_{R'}(\sigma_{R'})$ and $v'_R(\mu_R)$

$$\exp[v'(\mu)] = \sum_{\sigma_1, ..., \sigma_z} \exp\left[zv(\sigma) + p \sum_{i=1}^{z} \mu_i \sigma_i - u(\sigma, p)\right], \tag{3}$$

with $u(\sigma, p)$ given by

$$u(\sigma, p) = \ln(2 \cosh(ps_1)), \tag{4}$$

where $s_1 = \sum_{i=1}^{z} \sigma_i$ and p is a parameter. It follows from Eqs. (3) and (4) that $v'(\mu)$ and $v(\sigma)$ have the same symmetry properties with respect to the point group transfor-

mation of spins within the hypercube unit cell. Thus v and v' can be expressed in terms of the same invariant functions of Ising spins on the hypercube unit cell,

$$v(\sigma) = \sum_{i=0}^{l} K_i g_i(\sigma), \tag{5a}$$

$$v'(\mu) = \sum_{i=0}^{l} K'_i g_i(\mu), \tag{5b}$$

where $g_0(\sigma) = g_0(\mu) = 1$. The other g_i are defined and discussed in Appendix A. Let $\mathbf{K} = (K_0, K_1, ..., K_l)$ and $\mathbf{K}' = (K'_0, K'_1, ..., K'_l)$ denote vectors of the coupling constants. Equation (3) may be considered as a transformation of the coupling constants

$$\mathbf{K}' = \mathbf{F}(\mathbf{K}, P). \tag{6}$$

For z Ising spins on a hypercube unit cell, there are 2^z possible spin configurations and thus 2^z possible hypercube cell potentials $v'(\mu)$. However, many $v'(\mu)$ are equal due to the symmetries of the spins on a unit cell. In fact, the number of independent $v'(\mu)$ is the same as the number of independent coupling constants in Eq. (5), i.e., $l + 1$. Let $\mathbf{v}'$ denote the vector of these independent cell potentials $(v_1, v_2, ..., v_{l+1})$. Then v' is related to $K' = (K'_0, K'_1, ..., K'_l)$ by the linear transformation of the $(l + 1) \times (l + 1)$ matrix T,

$$(v'_1, v'_2, ..., v'_{l+1}) = (K'_0, K'_1, ..., K'_l)T, \tag{7}$$

or briefly denoted as

$$\mathbf{v}' = \mathbf{K}'T. \tag{8}$$

T can be calculated from Eq. (5). We also have the inverse transformation

$$\mathbf{K}' = \mathbf{v}'T^{-1}, \tag{9}$$

where $T^{-1}T = I$.

Now the free energy calculated from $H'(\mu_1, ..., \mu_{N'})$ is always a lower bound for the free energy calculated for $H(\sigma_1, \sigma_2, ..., \sigma_N)$ and we must vary p to obtain the optimum lower bound free energy. In the MKVM, the variational parameter p is determined by minimizing the single cell free energy. This leads to the nonlinear equation

$$\frac{\sum_{\mu_1, ..., \mu_z} (\partial v'/\partial p) \exp[v'(\mu)]}{\sum_{\mu_1, ..., \mu_z} \exp[v'(\mu)]} = 0, \tag{10}$$

which is solved at each iterative step to determine p. From Eqs. (3), (4) and (10), it is easy to show that Eq. (10) may be rewritten as

$$\frac{\sum_{i=1}^{l+1} D_i \exp(zv_i) \dfrac{d}{dp} F(s_{1,i}; p)}{\sum_{i=1}^{l+1} D_i \exp(zv_i) F(s_{1,i}; p)} = 0, \tag{11}$$

With $F(s_{1,i}; p)$ given by

$$F(s_{1,i}; p) = (2 \cosh p)^z / 2 \cosh(ps_{1,i}), \tag{12}$$

Where $s_{1,i}$ is $\sum_{j=1}^{z} \sigma_j$ evaluated at the ith degeneracy group. D_i and v_i are the number of elements and cell potential for the ith degeneracy group, respectively.

To begin with, we use $v_{R'}(\sigma_{R'})$ of Eq. (1) as $v(\sigma)$ in the right hand side of Eq. (3) with p given by Eq. (11) and calculate the cell potential $v'(\mu)$ from Eq. (3). This constitutes the first step of the RG transformation. We then use $v'(\mu)$ thus obtained as input in the same procedure to calculate the transformed potential $v''(\mu)$. This RG transformation is iterated further so that a series of cell potentials $v'(\mu)$, $v''(\mu)$,..., $v^{(\alpha)}(\mu)$ (and hence coupling constants K', K'',..., $K^{(\alpha)}$ and the corresponding variational parameters $p', p'', ..., p^{(\alpha)}$) are obtained. In this step-by-step RG transformation $K_i^{(\alpha)}$ for $i \geqslant 1$ and $p^{(\alpha)}$ tend to diminish to zero with increasing α when the system above the critical temperature and tend to grow when the system is below the critical temperature. Thus, after a large number, say α, of RG transformations, β times the free energy per spin for the original lattice may be approximated by

$$f^{(\alpha)} \simeq -\frac{1}{z^\alpha}(K_0^{(\alpha)} + \ln 2), \tag{13a}$$

for $T > T_c$ (or $\beta < \beta_c = 1/kT_c$) and

$$f^{(\alpha)} \simeq -\frac{1}{z^\alpha}\left[K_0^{(\alpha)} + \sum_{i=1}^{l} K_i^{(\alpha)} g_i(\boldsymbol{\sigma}_0)\right], \tag{13b}$$

for $T < T_c$ (or $\beta > \beta_c$), where $\boldsymbol{\sigma}_0$ is the spin configuration at $T = 0$.

To calculate the internal energy and spontaneous magnetization of the system, we must take the first derivative of $f^{(\alpha)}$ with respect to β and $h(=\beta B)$, respectively. Let q denote either β or h. By the chain rule, it is easy to see from Eq. (13) that

$$\frac{\delta f^{(\alpha)}}{\delta q} = -\frac{\delta \mathbf{K}^0}{\delta q} \circ \frac{\delta \mathbf{K}^{(1)}}{\delta \mathbf{K}^0} \cdots \frac{\delta \mathbf{K}^{(m)}}{\delta \mathbf{K}^{(m-1)}} \cdots \frac{\delta \mathbf{K}^{(\alpha)}}{\delta \mathbf{K}^{(\alpha-1)}} \frac{1}{z^\alpha} \mathbf{c}, \tag{14}$$

where

$$\mathbf{C} = (1, 0, ..., 0)^T, \tag{15a}$$

for $T > T_c$ and

$$\mathbf{C} = (1, g_1(\sigma_0), g_2(\sigma_0),..., g_l(\sigma_0))^T, \tag{15b}$$

for $T < T_c$.

It will become clear later that in order to deal with systems with different symmetry properties in a unified way, it is convenient to carry out the calculation in the cell potential space $v^{(\alpha)}(\mu)$ instead of the coupling constant space $K^{(\alpha)}$. From Eq. (8) and (9), we have

$$\frac{\delta \mathbf{K}^{(m)}}{\delta \mathbf{K}^{(m-1)}} = T \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} T^{-1}, \tag{16a}$$

$$\frac{\delta \mathbf{K}^{0}}{\delta q} = \frac{\delta \upsilon^{0}}{\delta q} T^{-1}. \tag{16b}$$

Thus Eq. (14) may be rewritten as

$$\frac{\delta f^{(\alpha)}}{\delta q} = -\frac{\delta \upsilon^{0}}{\delta q} \cdot \frac{\delta \upsilon^{(1)}}{\delta \upsilon^{0}} \cdots \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \cdots \frac{\delta \upsilon^{(\alpha)}}{\delta \upsilon^{(\alpha-1)}} \cdot \frac{1}{z^{\alpha}} T^{-1}\mathbf{C}. \tag{17}$$

In Appendix B, we derive very simple general formulas for $T^{-1}\mathbf{C}$ that allow us to avoid explicitly calculating the matrix T.

It should be noted that for $q = h$ in Eq. (14), $\mathbf{K}^{(m)}$ for $m = 1,..., \alpha$ must include all odd-spin coupling constants, even if we evaluate the row vector $\delta \mathbf{K}^{0}/\delta h$ and matrix $\delta \mathbf{K}^{(m)}/\delta \mathbf{K}^{(m-1)}$ at points where the odd spin coupling constants vanish. These points are equivalent to the points in the cell potential space with $v(\sigma_1,..., \sigma_z) = v(-\sigma_1,..., -\sigma_z)$. Thus to evaluate the spontaneous magnetization in cell potential space, we must consider $v(\sigma_1, \sigma_2,..., \sigma_z)$ and $v(-\sigma_1, -\sigma_2,..., -\sigma_z)$ as independent cell potentials.

To calculate the specific heat and susceptibility of the system, we must take the second derivative of $f^{(\alpha)}$ with respect to β and h. From Eq. (17), it follows that

$$\begin{aligned}
\frac{\delta^2 f^{(\alpha)}}{\delta q^2} = -\Bigg\{ & \frac{\delta^2 \upsilon^{0}}{\delta q^2} \cdot \frac{\delta \upsilon^{(1)}}{\delta \upsilon^{0}} \cdots \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \cdots \frac{\delta \upsilon^{(\alpha)}}{\delta \upsilon^{(\alpha-1)}} \\
& + \frac{\delta \upsilon^{0}}{\delta q} \cdot \frac{\delta^2 \upsilon^{(1)}}{\delta q\, \delta \upsilon^{0}} \cdots \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \cdots \frac{\delta \upsilon^{(\alpha)}}{\delta \upsilon^{(\alpha-1)}} \\
& + \cdots \\
& + \frac{\delta \upsilon^{0}}{\delta q} \cdot \frac{\delta \upsilon^{(1)}}{\delta \upsilon^{0}} \cdots \frac{\delta}{\delta q} \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \cdots \frac{\delta \upsilon^{(\alpha)}}{\delta \upsilon^{(\alpha-1)}} \\
& + \cdots \\
& \vdots \\
& + \frac{\delta \upsilon^{0}}{\delta q} \cdot \frac{\delta \upsilon^{(1)}}{\delta \upsilon^{0}} \cdots \frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \cdots \frac{\delta}{\delta q} \frac{\delta \upsilon^{(\alpha)}}{\delta \upsilon^{(\alpha-1)}} \Bigg\} \frac{1}{z^{\alpha}} T^{-1}\mathbf{C}.
\end{aligned} \tag{18}$$

By the chain rule

$$\frac{\delta}{\delta q}\cdot\frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}} \qquad \text{for } m=1,\ldots,\alpha$$

is further given by

$$\frac{\delta}{\delta q}\frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}}=\frac{\delta \upsilon^{0}}{\delta q}\cdot\frac{\delta \upsilon^{(1)}}{\delta \upsilon^{0}}\cdots\frac{\delta}{\delta \upsilon^{(m-1)}}\frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}}. \tag{19}$$

Thus to calculate $\delta f^{(\alpha)}/\delta q$ and $\delta^2 f^{(\alpha)}/\delta q^2$, we must evaluate $\delta \upsilon^0/\delta q$, $\delta^2 \upsilon^0/\delta q^2$, $\delta v_j^{(m)}/\delta v_i^{(m-1)}$ and $(\delta/\delta v_k^{(m-1)})(\delta v_j^{(m)}/\delta v_i^{(m-1)})$ for $i,\ j,\ k=1,\ldots,l+1$. It is straightforward to calculate the first two quantities from the initial cell potential of Eq. (1). From Eq. (3) we have

$$v_j^{(m)}=\ln\left[\sum_{\sigma}\exp\left(zv^{(m-1)}(\sigma)+p\sum_{k=1}^{z}\mu_k\sigma_k-u(\sigma,p)\right)\right], \tag{20}$$

where $(\mu_1,\ldots,\mu_z)$ is one of the spin configuration belonging to the jth degeneracy group and $u(\sigma,p)$ is given by Eq. (4). The variational parameter p of Eq. (20) is essentially determined by the initial cell potentials $v^{(m-1)}$. This fact must be taken into account in the calculation of $\delta v_j^{(m)}/\delta v_i^{(m-1)}$. Thus we have

$$\frac{\delta v_j^{(m)}}{\delta v_i^{(m-1)}}\equiv\left(\frac{\delta \upsilon^{(m)}}{\delta \upsilon^{(m-1)}}\right)_{ij}=\left(\frac{\partial v_j^{(m)}}{\partial v_i^{(m-1)}}\right)_p+\left(\frac{\partial v_j^{(m)}}{\partial p}\right)\left(\frac{\partial p}{\partial v_i^{(m-1)}}\right), \tag{21}$$

where

$$\left(\frac{\partial v_j^{(m)}}{\partial v_i^{(m-1)}}\right)_p=\frac{z\sum_{\sigma}'\exp[zv^{(m-1)}(\sigma)+p\sum_{k=1}^{z}\mu_k\sigma_k-u(\sigma,p)]}{\sum_{\sigma}\exp[zv^{(m-1)}(\sigma)+p\sum_{k=1}^{z}\mu_k\sigma_k-u(\sigma,p)]}, \tag{22}$$

$$\frac{\partial v_j^{(m)}}{\partial p}=\frac{\sum_{\sigma}\exp[zv^{(m-1)}(\sigma)+p\sum_{k=1}^{z}\mu_k\sigma_k-u(\sigma,p)]\left(\sum_{k=1}^{z}\mu_k\sigma_k-\dfrac{\partial}{\partial p}u\right)}{\sum_{\sigma}\exp[zv^{(m-1)}+p\sum_{k=1}^{z}\mu_k\sigma_k-u(\sigma,p)]}, \tag{23}$$

and

$$\frac{\partial p}{\partial v_i^{(m-)}}=-\frac{zD_i\exp(zv_i^{(m-1)})\dfrac{d}{dp}F(s_{1,i},p)}{\sum_{k=1}^{l+1}D_k\exp(zv_k^{(m-1)})\dfrac{d^2}{dp^2}F(s_{1,i},p)}, \tag{24}$$

where $F(s_{1,i};p)$ is given by Eq. (12). In Eq. (22), $\sum_{\sigma}'$ is a sum over all configurations of σ corresponding to the cell potential $v_i^{(m-1)}(\sigma)$. Equation (24) is derived from Eq. (11) and the notation is the same as that of Eq. (11).

From Eq. (21), it follows that

$$\frac{\delta^2 v_j^{(m)}}{\delta v_k^{(m-1)}\,\delta v_i^{(m-1)}} = \left(\frac{\partial v_j^{(m)}}{\partial v_k^{(m-1)}\,\partial v_i^{(m-1)}}\right)_p + \frac{\partial v_j^{(m)}}{\partial v_k^{(m-1)}\,\partial p}\,\frac{\partial p}{\partial v_i^{(m-1)}}$$

$$+ \frac{\partial v_j^{(m)}}{\partial p}\cdot\frac{\partial^2 p}{\partial v_k^{(m-1)}\,\partial v_i^{(m-1)}} \tag{25}$$

$$+ \left[\frac{\partial v_j^{(m)}}{\partial p\,\partial v_i^{(m-1)}} + \frac{\partial^2 v_j^{(m)}}{\partial p^2}\cdot\frac{\partial p}{\partial v_i^{(m-1)}} + \frac{\partial v_j^{(m)}}{\partial p}\cdot\frac{\partial}{\partial p}\,\frac{\partial p}{\partial v_i^{(m-1)}}\right]\frac{\partial p}{\partial v_k^{(m-1)}}.$$

It is straightforward to derive equations for the partial derivatives on the right side of Eq. (25). They are very involved so we do not report them here. It is obvious that Eq. (25) is symmetric with respect to the indices k and i. We have used this fact to check our expressions for the right hand side of Eq. (25).

This completes our formulation of the equations for the direct calculation of the first and second derivatives of the free energy.

III. Symmetry Properties

In order to carry out the configurational sum $\sum'$ in Eq. (22) and also the equations for the partial derivatives with respect to $v_k^{(m-1)}$ and $v_i^{(m-1)}$ on the right side of Eq. (25), we must establish the correspondence between spin configurations $(\sigma_1,\ldots,\sigma_z)$ and the independent cell potentials $v_i(\sigma_1,\ldots,\sigma_z)$. That is, we must classify the 2^z possible spin configurations into different groups, such that all configurations of the same group have the same cell potential $v_i(\sigma_1,\ldots,\sigma_z)$, where i runs from 1 to $l+1$. This correspondence depends on the space dimension and symmetry properties of the system. However, we can establish very simple general criteria for the purpose of such configuration classification.

In Appendix A, we list invariant functions for certain systems in one to three dimensions. We also list the relations between invariants of a given system. From such relations, it is easy to see that all inveriants for a given system may be expressed in terms of certain basic invariants. These are also given Table I. Thus by Eq. (5), any cell potential $v(\sigma_1,\ldots,\sigma_z)$ can be expressed as a function of these basic invariants. So we may use these basic invariants as criteria to classify the spin configurations. The generation of all possible configurations and their classification into different groups based on their basic invariants may be carried out simply by computer. This scheme is briefly described in Appendix B.

In Table I, we also list the values of $l+1$ and possible applications of the considered models.

TABLE I

Basic Invariants and Possible Applications for the Considered Models

Model	Dimension	Basic invariants	$l+1$	Application[a]
S_1	1	g_1	3	
S_2	2	g_1	5	Isotropic SQ lattice with nn interaction only.
S_3	2	g_1, g_2	6	Isotropic SQ lattice with nn, nnn and 4 spin interactions.
S_4	2	g_1, g_2, g_3	7	Anisotropic SQ lattice with nn, nnn, and 4 spin interactions.
S_5	2	g_1, g_2	9	Triangular lattice with nn and nnn interactions.
S_6	3	g_1	9	Isotropic BCC lattice with nn interaction only.
S_7	3	g_1, g_2, g_3	22	Isotropic SC lattice with all possible even spin interactions within the primitive unit cell.
S_8	3	g_1, g_2, g_3, g_4, g_5	34	Anisotropic SC (tetragonal) lattice. Crossover from $d=2$ to $d=3$.
S_9	3	g_1, g_2, g_3, g_4, g_5	46	Isotropic FCC lattice with all possible even spin interactions within the primitive unit cell.

Note. The definition of g_i (see Appendix A) may differ from case to case.
[a] nn = Nearest neighbor; nnn = next nearest neighbor.

IV. An Example: Permutation Symmetry

In this section, we apply the formalism developed in the previous sections to an Ising model with isotropic nearest neighbor interactions on one-dimensional, two-dimensional square, and three-dimensional body-centered cubic lattices. The Hamiltonian in these cases may be written as

$$\beta H = -k \sum_{(nn)} \sigma_i \sigma_j - h \sum_i \sigma_i \equiv -\sum_R v_R, \tag{26a}$$

$$v_R = k\sigma_c(\sigma_1 + \cdots + \sigma_z) + \frac{h}{z}(\sigma_1 + \cdots + \sigma_z) + h\sigma_c, \tag{26b}$$

where R is a unit cell with one spin σ_c in the center, z spins $\sigma_1,\ldots,\sigma_z$ at the corners and the factor $\beta(=1/kT)$ has already been included in K and h. Performing a

a
$-\frac{\delta f}{\delta K}$
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K
b
$-\frac{\delta^2 f}{\delta K^2}$
0.00
40.00
80.00
120.00
160.00
200.00
240.00
280.00
320.00
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K

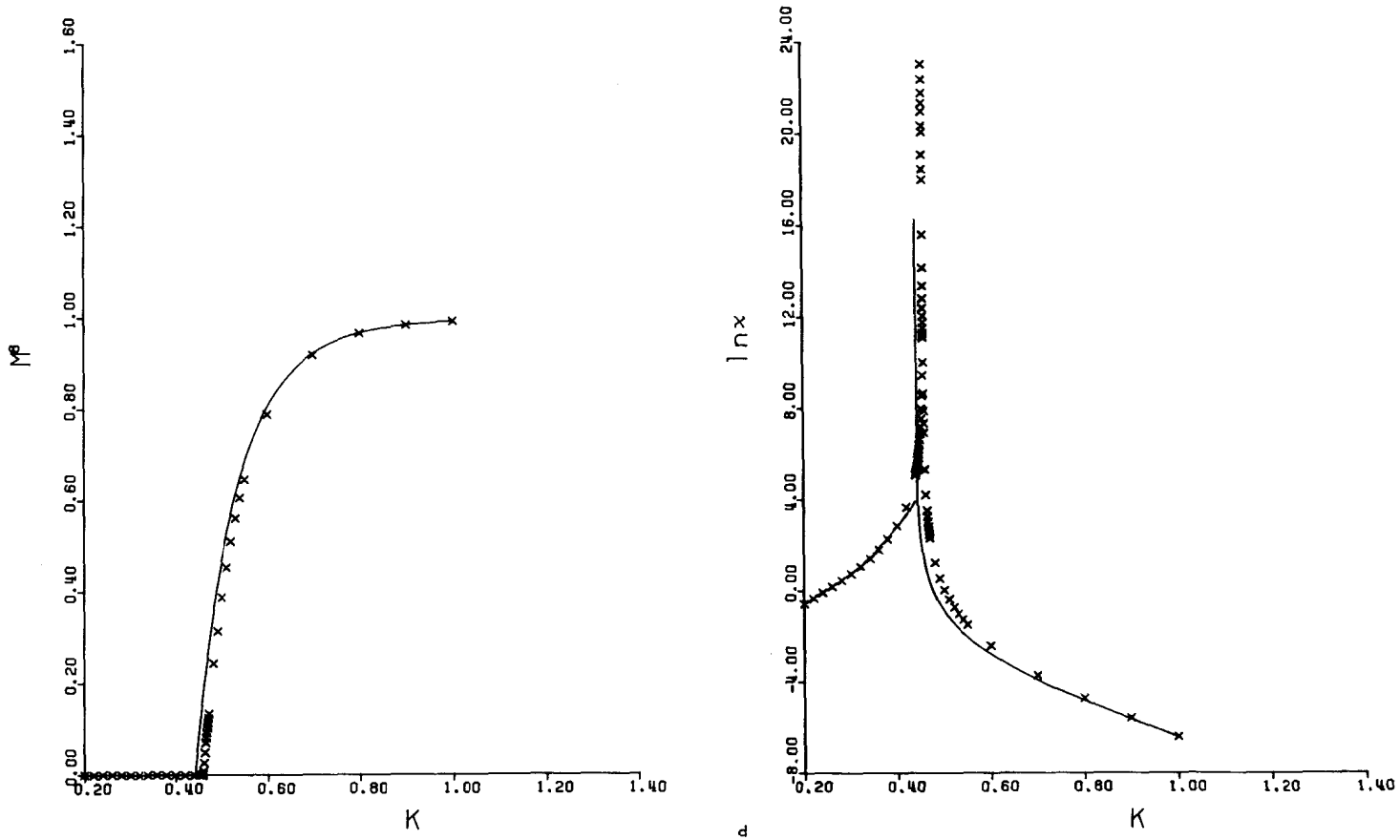

FIG. 1. Derivatives of the free energy for the Ising Model on the SQ lattice. (a) $-\delta f/\delta k$ as function of K. (b) $-\delta^2 f/\delta K^2$ as function of K. (c) M^8 as function of K, where $M = -\delta f/\delta h$. (d) $\ln \chi$ as a function of K, where $\chi = -K(\delta^2 f/\delta^2 h)$. The solid curves in Figs. 1a, b and c represent Onsager's [9] or Yang's [10] exact solution. The solid curve in Fig. 1d is obtained from high temperature [12] and low temperature [11] series expansion.

a
$-\frac{\delta f}{\delta K}$
0.00
0.40
0.60
0.80
1.00
1.20
1.40
1.60
1.80
2.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K
b
$-\frac{\delta^2 f}{\delta K^2}$
0.00
4.00
8.00
12.00
16.00
20.00
24.00
28.00
32.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K

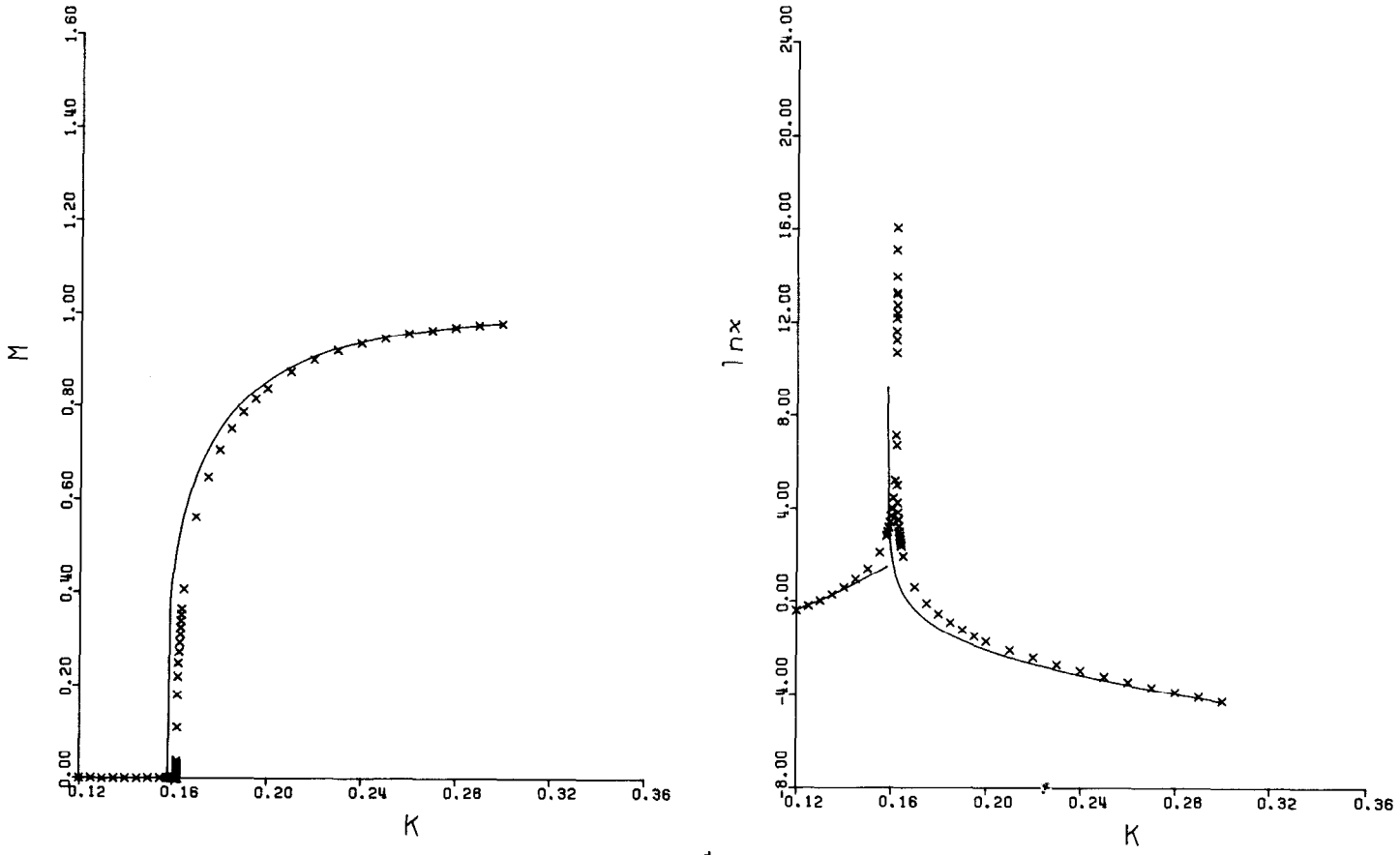

FIG. 2. Derivatives of the free energy for the Ising model on the *BCC* lattice. (a) $-\delta f/\delta k$ as function of K. (b) $-\delta^2 f/\delta k^2$ as function of K. (c) M as a function of k, where $M = -\delta f/\delta h$. (d) $\ln \chi$ as a function of k, where $\chi = -k(\delta^2 f/\delta^2 h)$. The solid curves are obtained from high temperature [12] or low temperature [11] series expansion.

decimation calculation which sums over the central spin in each cell, we obtain an effective Hamiltonian for the remaining spins. The resulting cell potential is

$$v_{\text{eff},R} = \frac{h}{z}(\sigma_1 + \cdots + \sigma_z) + \ln 2 \cosh(h + k(\sigma_1 + \cdots + \sigma_z)), \tag{27}$$

which has permutation symmetry with respect to σ_1, σ_2,..., σ_z and thus according to Appendix A can be classified as $S1$, $S2$ or $S6$ for d equal to 1, 2 or 3, respectively. We can use $g_1 = \sigma_1 + \cdots + \sigma_z$ as the basic invariant to classify the 2^z possible configurations of σ_1,..., σ_z into different degeneracy groups, each of which corresponds to the same cell potential. We then use $v_{\text{eff},R}$ of Eq. (27) as v_0 in Section II to calculate the free energy per spin and its first and second derivatives with respect to K and h. We must divide all these quantities by a factor 2 because Eq. (27) was obtained after a decimation calculation. The results for $d = 1$ agree extremely well with the exact results obtained by transfer matrix method [13]. These results also provide a check on our computer program.

A few results for $d = 2$ and 3 are shown in Figs. 1 and 2, respectively. Figs. 1b and c should be compared with Figs. 6 and 7 in the paper by Kadanoff *et al.* [1]. Their results were obtained by numerical differentiation for the free energy and thus involve more numerical error than the present work.

In future work, we will present the results of this method applied to several models with different symmetry properties. Preliminary analysis indicates that we obtain very accurate values both close to and far from the transition temperature, as is clear from Figs. 1 and 2. The application of this method near the transition temperature is of particular interest since it allows an evaluation of correction-to-scaling effects due to nonlinear terms and all the (linearized renormalization group) eigenvalues.

V. Discussion

From the previous sections, it is clear that to calculate the free energy and its derivatives for a given model, it is sufficient to use the basic invariants of the model, and not necessary to use the relations among all invariants (i.e., the even numbered equations of Appendix A). For a given system, it is much easier to obtain the former than the latter. However, if we desire to calculate the flow of the coupling constants $(K_1, K_2,..., K_l)$ in parameter space, as the step-by-step RG transformation is carried out, we may use the even numbered equations of Appendix A to calculate the $(l+1) \times (l+1)$ matrix T, and hence T^{-1} of Eqs. (8) and (9), respectively.

The method used in this paper may be easily extended and applied to systems with symmetry properties different from those listed in Table I. In particular, we may combine the ideas of this paper and our previous work [14] to calculate derivatives of the free energy for antiferromagnetic systems.

It is clear from the preceding sections that to write a single computer program applicable to many systems with different symmetry properties, it is very convenient

to carry out the calculation in cell potential space. Some of the calculation techniques in this paper may be combined with other RG transformation methods, such as Nauenberg and Nienhuis' method [15], to calculate the free energies and their derivatives.

Our approximate method to determine the variational parameters in the lower bound RG transformation of Kadanoff *et al.* is not a full implementation of the variational principle. This is because we determine the variational parameters by minimizing the free energy of a single cell, which has a finite number of spins. Thus the variational parameters are uncoupled from the singularities of the free energy of the system and we do not encounter the singularity problem considered by Van Saarloos *et al.* [16] den Nijs and Knops [17] and Barber [18].

APPENDIX A: SYMMETRY PROPERTIES AND INVARIANT FUNCTIONS FOR ISING SPINS ON HYPERCUBE UNIT CELL

The locations of the z $(=2^d)$ Ising spins on a hypercube unit cell are shown in Figs. A1, A2 and A3 for $d = 1$, 2 and 3, respectively. We shall use K_{ij} to denote the two-spin coupling constant between σ_i and σ_j which appears on the right hand side of Eq. (5).

Now we consider and write down the invariant functions on the right hand side of Eq. (5) for the following possible systems.

$S1$: $d = 1$.

$$\begin{aligned} g_1 &= \sigma_1 + \sigma_2, \\ g_2 &= \sigma_1 \sigma_2. \end{aligned} \tag{A1}$$

They satisfy the relation

$$g_2 = g_1^2/2 - 1. \tag{A2}$$

$S2$: $d = 2$; $v(\sigma_1,..., \sigma_4)$ has permutation symmetry.

$$\begin{aligned} g_1 &= \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4, \\ g_2 &= \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 + \sigma_1\sigma_3 + \sigma_2\sigma_4, \\ g_3 &= \sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2, \\ g_4 &= \sigma_1\sigma_2\sigma_3\sigma_4. \end{aligned} \tag{A3}$$

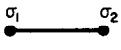

FIG. A1. Location of the Ising spins σ_1, σ_2 on the one-dimensional unit cell.

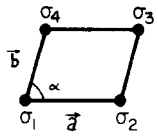

FIG. A2. Location of the Ising spins σ_1, σ_2, σ_3, σ_4 on the two-dimensional unit cell. **a** and **b** are the primitive translation vectors and α is the angle between them.

They satisfy the relations

$$\begin{aligned} g_2 &= g_1^2/2 - 2, \\ g_3 &= [g_1 g_2 - 3g_1]/3, \\ g_4 &= [g_1 g_3 - 2g_2]/4. \end{aligned} \tag{A4}$$

$S3$: $d=2$; $v(\sigma_1,\ldots,\sigma_4)$ has rotation, reflection and inversion symmetries. $K_{12}=K_{23}=K_{34}=K_{41}$, $K_{13}=K_{24}$, but $K_{12}\neq K_{13}$. For the unit cell of Fig. A2, $|\mathbf{a}|=|\mathbf{b}|$, $\alpha=90°$

$$\begin{aligned} g_1 &= \sigma_1+\sigma_2+\sigma_3+\sigma_4, \\ g_2 &= \sigma_1\sigma_3+\sigma_2\sigma_4, \\ g_3 &= \sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1, \\ g_4 &= \sigma_1\sigma_2\sigma_3+\sigma_2\sigma_3\sigma_4+\sigma_3\sigma_4\sigma_1+\sigma_4\sigma_1\sigma_2, \\ g_5 &= \sigma_1\sigma_2\sigma_3\sigma_4. \end{aligned} \tag{A5}$$

They satisfy the relations

$$\begin{aligned} g_3 &= g_1^2/2 - g_2 - 2, \\ g_4 &= g_1 g_2 - g_1 \\ g_5 &= g_2^2/2 - 1. \end{aligned} \tag{A6}$$

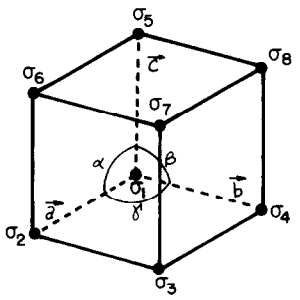

FIG. A3. Location of the Ising spins σ_1, σ_2,..., σ_8 on the three-dimensional unit cell. **a**, **b**, and **c** are the primitive translation vectors and α, β, γ are the angles between them.

$S4$: $d=2$; $v(\sigma_1,...,\sigma_4)$ has reflection and inversion symmetries. $K_{12}=K_{34}$, $K_{23}=K_{41}$, $K_{12}\neq K_{23}$, $K_{13}=K_{24}$. For the unit cell of Fig. A2, $|\mathbf{a}|\neq|\mathbf{b}|$, $\alpha=90°$.

$$\begin{aligned} g_1 &= \sigma_1+\sigma_2+\sigma_3+\sigma_4,\\ g_2 &= \sigma_1\sigma_3+\sigma_2\sigma_4,\\ g_3 &= \sigma_1\sigma_2+\sigma_3\sigma_4,\\ g_4 &= \sigma_1\sigma_4+\sigma_2\sigma_3,\\ g_5 &= \sigma_1\sigma_2\sigma_3+\sigma_2\sigma_3\sigma_4+\sigma_3\sigma_4\sigma_1+\sigma_4\sigma_1\sigma_2,\\ g_6 &= \sigma_1\sigma_2\sigma_3\sigma_4. \end{aligned} \tag{A7}$$

They satisfy the relations

$$\begin{aligned} g_4 &= g_1^2/2-g_2-g_3-2,\\ g_5 &= g_1g_2-1,\\ g_6 &= g_2^2/2-1. \end{aligned} \tag{A8}$$

$S5$: $d=2$; $v(\sigma_1,...,\sigma_4)$ has inversion symmetry. $K_{12}=K_{23}=K_{34}=K_{41}$, $K_{13}\neq K_{24}$ for the unit cell of Fig. A2, $|\mathbf{a}|=|\mathbf{b}|$, $\alpha=60°$.

$$\begin{aligned} g_1 &= \sigma_1+\sigma_3,\\ g_2 &= \sigma_2+\sigma_4,\\ g_3 &= \sigma_1\sigma_3,\\ g_4 &= \sigma_2\sigma_4,\\ g_5 &= \sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1,\\ g_6 &= \sigma_1\sigma_2\sigma_3+\sigma_1\sigma_3\sigma_4,\\ g_7 &= \sigma_1\sigma_2\sigma_4+\sigma_2\sigma_3\sigma_4,\\ g_8 &= \sigma_1\sigma_2\sigma_3\sigma_4. \end{aligned} \tag{A9}$$

They satisfy the relations

$$\begin{aligned} g_3 &= g_1^2/2-1,\\ g_4 &= g_2^2/2-1,\\ g_5 &= g_1g_2,\\ g_6 &= g_2g_3,\\ g_7 &= g_1g_4,\\ g_8 &= g_3g_4. \end{aligned} \tag{A10}$$

$S6$: $d = 3$; $v(\sigma_1,..., \sigma_8)$ has permutation symmetry.

Let g_i denote the sum of all possible products of i different σ's. g_i, for $i = 1,..., 8$, are the basic invariants of the permutation group. It is easy to show that g_i satisfy the relation

$$g_1 = \sigma_1 + \sigma_2 + \cdots + \sigma_8, \tag{A11}$$

$$g_{i+1} = [g_1 g_i - (8 - i + 1) g_{i-1}]/(i + 1), \tag{A12}$$

for $i = 1,..., 7$. Thus each g_i may be expressed in terms of g_1.

$S7$: $d = 3$; $v(\sigma_1,..., \sigma_8)$ of Eq. (5) has symmetry properties of the simple cubic unit cell, i.e., 0_h point group.

$$\begin{aligned}
g_1 &= \sigma_1 + \sigma_2 + \sigma_3 + \cdots + \sigma_8, \\
g_2 &= \sigma_1\sigma_2 + \cdots && \text{(12 terms)}, \\
g_3 &= \sigma_1\sigma_7 + \cdots && \text{(4 terms)}, \\
g_4 &= \sigma_1\sigma_3 + \cdots && \text{(12 terms)}, \\
g_5 &= \sigma_1\sigma_2\sigma_3\sigma_4 + \cdots && \text{(6 terms)}, \\
g_6 &= \sigma_1\sigma_2\sigma_3\sigma_8 + \cdots && \text{(24 terms)}, \\
g_7 &= \sigma_1\sigma_2\sigma_3\sigma_6 + \cdots && \text{(8 terms)}, \\
g_8 &= \sigma_1\sigma_2\sigma_3\sigma_7 + \cdots && \text{(24 terms)}, \\
g_9 &= \sigma_1\sigma_2\sigma_7\sigma_8 + \cdots && \text{(6 terms)}, \\
g_{10} &= \sigma_1\sigma_3\sigma_6\sigma_8 + \cdots && \text{(2 terms)}, \\
g_{11} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots && \text{(12 terms)}, \\
g_{12} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7 + \cdots && \text{(12 terms)}, \\
g_{13} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8 + \cdots && \text{(4 terms)}, \\
g_{14} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8 && \text{(1 term)}, \\
g_{15} &= \sigma_1\sigma_2\sigma_3 + \cdots && \text{(24 terms)}, \\
g_{16} &= \sigma_1\sigma_2\sigma_7 + \cdots && \text{(24 terms)}, \\
g_{17} &= \sigma_1\sigma_3\sigma_6 + \cdots && \text{(8 terms)}, \\
g_{18} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5 + \cdots && \text{(24 terms)}, \\
g_{19} &= \sigma_1\sigma_2\sigma_3\sigma_7\sigma_8 + \cdots && \text{(24 terms)}, \\
g_{20} &= \sigma_1\sigma_3\sigma_4\sigma_6\sigma_8 + \cdots && \text{(8 terms)}, \\
g_{21} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7 + \cdots && \text{(8 terms)},
\end{aligned} \tag{A13}$$

where, in order to save space, only one typical term for each invariant is written. It is easy to show that the g_i of Eq. (A13) are related to each other by the equations

$$
\begin{aligned}
g_4 &= g_1^2/2 - g_2 - g_3 - 4, \\
g_6 &= g_3\, g_4 - 2g_2, \\
g_8 &= g_2\, g_3 - 2g_4, \\
g_9 &= g_3^2/2 - 2, \\
g_5 &= (g_2^2/2 - 6 - 2g_4 - g_8 - g_9)/2, \\
g_7 &= (g_2\, g_4 - 4g_2 - 6g_3 - 2g_6)/3, \\
g_{10} &= g_4^2/6 - 2 - \tfrac{2}{3} g_4 - g_5/3 - g_8/3 - g_9/3, \\
g_{14} &= g_{10}^2/2 - 1, \\
g_{11} &= g_2\, g_{14}, \\
g_{12} &= g_4\, g_{14}, \\
g_{13} &= g_3\, g_{14}, \\
g_{16} &= g_1\, g_3 - g_1, \\
g_{15} &= (g_1\, g_2 - 3g_1 - g_{16})/2, \\
g_{17} &= (g_1\, g_4 - 3g_1 - g_{15} - g_{16})/3, \\
g_{18} &= g_{14}\, g_{15}, \\
g_{19} &= g_{14}\, g_{16}, \\
g_{20} &= g_{14}\, g_{17}, \\
g_{21} &= g_{14}\, g_1.
\end{aligned}
\tag{A14}
$$

S8: $d = 3$; $v(\sigma_1, \sigma_2, \ldots, \sigma_8)$ of Eq. (5) has symmetry properties of the tetragonal unit cell. For the unit cell of Fig. A3, $|\mathbf{a}| = |\mathbf{b}| \neq |\mathbf{c}|$, $\alpha = \beta = \gamma = 90°$.

$$
\begin{aligned}
g_1 &= \sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 + \sigma_6 + \sigma_7 + \sigma_8, \\
g_2 &= \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 + \sigma_5\sigma_6 + \sigma_6\sigma_7 + \sigma_7\sigma_8 + \sigma_8\sigma_1, \\
g_3 &= \sigma_1\sigma_5 + \sigma_2\sigma_6 + \sigma_3\sigma_7 + \sigma_4\sigma_8, \\
g_4 &= \sigma_1\sigma_7 + \sigma_2\sigma_8 + \sigma_3\sigma_5 + \sigma_4\sigma_6, \\
g_5 &= \sigma_1\sigma_3 + \sigma_2\sigma_4 + \sigma_5\sigma_7 + \sigma_6\sigma_8, \\
g_6 &= \sigma_1\sigma_6 + \sigma_2\sigma_5 + \sigma_2\sigma_7 + \sigma_3\sigma_6 + \sigma_3\sigma_8 + \sigma_4\sigma_7 + \sigma_1\sigma_8 + \sigma_4\sigma_5, \\
g_7 &= \sigma_1\sigma_2\sigma_3\sigma_4 + \sigma_5\sigma_6\sigma_7\sigma_8,
\end{aligned}
$$

$$
\begin{aligned}
g_8 &= \sigma_1\sigma_2\sigma_6\sigma_5 + \sigma_2\sigma_3\sigma_7\sigma_6 + \sigma_3\sigma_4\sigma_8\sigma_7 + \sigma_1\sigma_4\sigma_5\sigma_8, \\
g_9 &= \sigma_1\sigma_2\sigma_3\sigma_8 + \cdots \quad (8 \text{ terms}) \\
g_{10} &= \sigma_1\sigma_2\sigma_6\sigma_8 + \cdots \quad (16 \text{ terms}) \\
g_{11} &= \sigma_1\sigma_2\sigma_3\sigma_6 + \cdots \quad (8 \text{ terms}) \\
g_{12} &= \sigma_1\sigma_2\sigma_3\sigma_7 + \cdots \quad (16 \text{ terms}) \\
g_{13} &= \sigma_1\sigma_2\sigma_6\sigma_7 + \cdots \quad (8 \text{ terms}) \\
g_{14} &= \sigma_1\sigma_2\sigma_7\sigma_8 + \cdots \quad (4 \text{ terms}) \\
g_{15} &= \sigma_1\sigma_5\sigma_3\sigma_7 + \sigma_2\sigma_6\sigma_4\sigma_8, \\
g_{16} &= \sigma_1\sigma_3\sigma_6\sigma_8 + \sigma_2\sigma_4\sigma_5\sigma_7, \\
g_{17} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots \quad (8 \text{ terms}), \\
g_{18} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_6\sigma_7 + \cdots \quad (4 \text{ terms}), \\
g_{19} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8 + \cdots \quad (4 \text{ terms}), \\
g_{20} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7 + \cdots \quad (4 \text{ terms}), \\
g_{21} &= \sigma_1\sigma_2\sigma_4\sigma_5\sigma_6\sigma_7 + \cdots \quad (8 \text{ terms}), \\
g_{22} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8, \\
g_{23} &= \sigma_1\sigma_2\sigma_3 + \cdots \quad (8 \text{ terms}), \\
g_{24} &= \sigma_1\sigma_2\sigma_6 + \cdots \quad (16 \text{ terms}), \\
g_{25} &= \sigma_1\sigma_2\sigma_7 + \cdots \quad (16 \text{ terms}), \\
g_{26} &= \sigma_1\sigma_5\sigma_3 + \cdots \quad (8 \text{ terms}), \\
g_{27} &= \sigma_1\sigma_3\sigma_6 + \cdots \quad (8 \text{ terms}), \\
g_{28} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5 + \cdots \quad (8 \text{ terms}), \\
g_{29} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_6 + \cdots \quad (16 \text{ terms}), \\
g_{30} &= \sigma_1\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots \quad (16 \text{ terms}), \\
g_{31} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_7 + \cdots \quad (8 \text{ terms}), \\
g_{32} &= \sigma_1\sigma_2\sigma_3\sigma_6\sigma_8 + \cdots \quad (8 \text{ terms}), \\
g_{33} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7 + \cdots \quad (8 \text{ terms}),
\end{aligned}
\tag{A15}
$$

where in order to save space, only one typical term for some invariants is written. Invariants of Eq. (A15) satisfy the relations

$$g_6 = g_1^2/2 - g_2 - g_3 - g_4 - g_5 - 4,$$

$$
\begin{aligned}
g_9 &= g_4 g_5 - 2g_3, \\
g_{10} &= g_4 g_6 - 2g_2, \\
g_{11} &= g_3 g_5 - 2g_4, \\
g_{12} &= g_2 g_3 - 2g_6, \\
g_{13} &= g_3 g_4 - 2g_5, \\
g_{16} &= (g_5^2 + g_6^2 - 4 - g_{13} - 2g_5 - g_4^2/2 - g_2^2/2 - g_3^2/2)/6, \\
g_7 &= (g_2^2 + 4g_{16} - g_6^2)/4, \\
g_{15} &= g_5^2/2 - 2 - g_7 - g_{16}, \\
g_8 &= g_3^2/2 - 2 - g_{15}, \\
g_{14} &= g_4^2/2 - 2 - g_{15}, \\
g_{22} &= g_7^2/2 - 1, \\
g_i &= g_{22} g_{i-15} \qquad \text{for} \quad i = 17,\ldots, 21, \\
g_{23} &= g_1(2g_2 - g_3 - g_4 + 2g_5 - g_6 - 2)/6, \\
g_{24} &= 2g_{23} - g_1(g_2 - g_6 + 2g_5 - 2g_4)/2, \\
g_{25} &= 2g_{23} - g_1(g_2 - g_6 + 2g_5 - 2g_4)/2, \\
g_{26} &= -2g_{23} + g_1(g_2 - g_6 + 2g_5 - 2)/2, \\
g_{27} &= g_{23} - g_1(g_2 - g_6)/2, \\
g_i &= g_{22} g_{i-5} \qquad \text{for} \quad i = 28, 29,\ldots, 32, \\
g_{33} &= g_{22} g_1 .
\end{aligned}
\tag{A16}
$$

$S9$: $d = 3$; $v(\sigma_1,\ldots,\sigma_8)$ has the symmetry properties of the primitive unit cell for the FCC lattice. The longest diagonal is in the σ_1, σ_7 direction. For the unit cell of Fig. A3, $|\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}|$, $\alpha = \beta = \gamma = 60°$.

$$
\begin{aligned}
g_1 &= \sigma_1 + \sigma_7, \\
g_2 &= \sigma_2 + \sigma_4 + \sigma_5 + \sigma_3 + \sigma_6 + \sigma_8, \\
g_3 &= \sigma_2\sigma_4 + \sigma_4\sigma_5 + \sigma_2\sigma_5 + \sigma_3\sigma_6 + \sigma_3\sigma_8 + \sigma_6\sigma_8, \\
g_4 &= \sigma_1(\sigma_3 + \sigma_6 + \sigma_8) + \sigma_7(\sigma_2 + \sigma_4 + \sigma_5), \\
g_5 &= \sigma_2\sigma_8 + \sigma_3\sigma_5 + \sigma_4\sigma_6, \\
g_6 &= \sigma_1\sigma_7, \\
g_7 &= \sigma_1(\sigma_2 + \sigma_4 + \sigma_5) + \sigma_7(\sigma_3 + \sigma_6 + \sigma_8), \\
g_8 &= \sigma_2\sigma_3 + \sigma_2\sigma_6 + \sigma_5\sigma_6 + \sigma_5\sigma_8 + \sigma_4\sigma_8 + \sigma_3\sigma_4,
\end{aligned}
$$

$$
\begin{aligned}
g_9 &= \sigma_1\sigma_2\sigma_3\sigma_4 + \cdots \quad \text{(6 terms)},\\
g_{10} &= \sigma_1\sigma_2\sigma_3\sigma_8 + \cdots \quad \text{(12 terms)},\\
g_{11} &= \sigma_1\sigma_2\sigma_4\sigma_7 + \cdots \quad \text{(6 terms)},\\
g_{12} &= \sigma_2\sigma_3\sigma_6\sigma_8 + \cdots \quad \text{(6 terms)},\\
g_{13} &= \sigma_1\sigma_2\sigma_3\sigma_6 + \cdots \quad \text{(6 terms)},\\
g_{14} &= \sigma_1\sigma_2\sigma_4\sigma_5 + \sigma_3\sigma_6\sigma_7\sigma_8,\\
g_{15} &= \sigma_1\sigma_2\sigma_3\sigma_7 + \cdots \quad \text{(6 terms)},\\
g_{16} &= \sigma_2\sigma_3\sigma_4\sigma_8 + \cdots \quad \text{(6 terms)},\\
g_{17} &= \sigma_2\sigma_3\sigma_7\sigma_8 + \cdots \quad \text{(12 terms)},\\
g_{18} &= \sigma_1\sigma_2\sigma_7\sigma_8 + \sigma_1\sigma_4\sigma_6\sigma_7 + \sigma_1\sigma_5\sigma_3\sigma_7,\\
g_{19} &= \sigma_3\sigma_4\sigma_5\sigma_6 + \sigma_2\sigma_3\sigma_5\sigma_8 + \sigma_2\sigma_6\sigma_4\sigma_8,\\
g_{20} &= \sigma_1\sigma_3\sigma_6\sigma_8 + \sigma_2\sigma_4\sigma_5\sigma_7,\\
g_{21} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7 + \cdots \quad \text{(6 terms)},\\
g_{22} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_6\sigma_8 + \cdots \quad \text{(6 terms)},\\
g_{23} &= \sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8 + \cdots \quad \text{(3 terms)} \qquad \text{(A17)}\\
g_{24} &= \sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_8,\\
g_{25} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots \quad \text{(6 terms)}\\
g_{26} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_6\sigma_7 + \cdots \quad \text{(6 terms)}\\
g_{27} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8\\
g_{28} &= \sigma_1\sigma_2\sigma_4 + \cdots \quad \text{(6 terms)},\\
g_{29} &= \sigma_2\sigma_3\sigma_6 + \cdots \quad \text{(6 terms)},\\
g_{30} &= \sigma_1\sigma_2\sigma_6 + \cdots \quad \text{(12 terms)},\\
g_{31} &= \sigma_1\sigma_7(\sigma_2 + \sigma_4 + \sigma_5 + \sigma_3 + \sigma_6 + \sigma_8),\\
g_{32} &= \sigma_1\sigma_2\sigma_8 + \cdots \quad \text{(6 terms)},\\
g_{33} &= \sigma_2\sigma_6\sigma_8 + \cdots \quad \text{(12 terms)},\\
g_{34} &= \sigma_1\sigma_3\sigma_6 + \cdots \quad \text{(6 terms)},\\
g_{35} &= \sigma_3\sigma_6\sigma_8 + \sigma_2\sigma_4\sigma_5,\\
g_{36} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5 + \cdots \quad \text{(6 terms)}\\
g_{37} &= \sigma_1\sigma_2\sigma_3\sigma_4\sigma_7 + \cdots \quad \text{(6 terms)}
\end{aligned}
$$

$$g_{38} = \sigma_1\sigma_2\sigma_3\sigma_4\sigma_6 + \cdots \qquad (12 \text{ terms}),$$
$$g_{39} = \sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots \qquad (6 \text{ terms}),$$
$$g_{40} = \sigma_1\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots \qquad (6 \text{ terms}),$$
$$g_{41} = \sigma_1\sigma_3\sigma_4\sigma_5\sigma_7 + \cdots \qquad (12 \text{ terms}),$$
$$g_{42} = \sigma_1\sigma_2\sigma_3\sigma_6\sigma_8 + \cdots \qquad (6 \text{ terms}),$$
$$g_{43} = \sigma_1\sigma_2\sigma_4\sigma_5\sigma_7 + \sigma_1\sigma_3\sigma_6\sigma_8\sigma_7,$$
$$g_{44} = \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_8 + \sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8,$$
$$g_{45} = \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7 + \cdots \qquad (6 \text{ terms}),$$

where in order to save space, only one typical term for some invariants is written. Invariants of Eq. (A15) satisfy the relations

$$\begin{aligned}
g_6 &= g_1^2/2 - 1,\\
g_7 &= g_1 g_2 - g_4,\\
g_8 &= g_2^2/2 - 3 - g_3 - g_5,\\
g_{10} &= g_4 g_5 - g_7,\\
g_{11} &= g_3 g_6,\\
g_{12} &= g_3 g_5 - 2g_8,\\
g_{13} &= g_4 g_8/2 - g_7 - g_{10},\\
g_{14} &= (g_3 g_7 - 2g_7 - g_{13} - g_{10})/3,\\
g_{15} &= g_6 g_8,\\
g_{18} &= g_5 g_6,\\
g_{19} &= (g_5^2 - 3)/2,\\
g_{16} &= g_3^2/2 - 3 - g_3 - g_{19},\\
g_{17} &= (g_7 + g_8)(g_5 + g_6) - 2(g_3 + g_4) - g_{15} - g_{16},\\
g_9 &= g_7 g_8/2 - g_4 - g_{17}/2,\\
g_{20} &= (g_3 g_4 - 2g_4 - g_{17} - g_9)/3,\\
g_{27} &= g_{20}^2/2 - 1,\\
g_i &= g_{27} g_{i-18} \qquad \text{for} \quad i = 21, 22, \ldots, 26,\\
g_{30} &= g_1 g_8,\\
g_{31} &= g_2 g_6,\\
g_{32} &= g_1 g_5,
\end{aligned} \tag{A18}$$

$$g_{33} = g_2 g_5 - g_2,$$
$$g_{34} = (g_2 g_4 - 3g_1 - g_{30} - g_{32})/2,$$
$$g_{28} = g_1 g_3 - g_{34},$$
$$g_{29} = (g_2 g_8 - 2g_2 - g_{33})/2,$$
$$g_{35} = (g_2 g_3 - 2g_2 - g_{29} - g_{33})/3,$$
$$g_i = g_{27} g_{i-8} \quad \text{for } i = 36, 37, \ldots, 43,$$
$$g_i = g_{27} g_{i-43} \quad \text{for } i = 44, 45.$$

APPENDIX B: DETAILS OF THE CALCULATION

In this appendix, we outline some techniques used in our computer program to obtain the numerical results. Our computer program can be applied to all systems listed in Appendix A with space dimension and symmetry properties as input parameters. The important programming techniques are as follows:

1. *Generation of all possible spin configurations.* Let z denote the number of spins on a hypercube unit cell of the d dimensional lattice and NCF denote the number of all possible configuration of such z spins $\sigma_1, \ldots, \sigma_z$; then $z = 2^d$, $NCF = 2^z$. Let I be an integer running from 0 to $NCF - 1$. We express I as a z digit binary number and let 1 correspond to spin up $(+1)$ and 0 correspond spin down (-1); then each binary integer from 0 to $NCF - 1$ corresponds to a spin configuration (e.g., the integer 0 corresponds to all spins down and $NCF - 1$ corresponds to all spins up, which is the ground state of the ferromagnetic system). Thus, with d as input parameter, we can generate all possible spin configurations.[1]

2. *Classification of spin configurations.* From Table I, it is clear that for space dimension $d \geqslant 2$ there are systems that have different symmetry properties. Thus, for each spin configuration generated in the manner described above, we calculate the values of the basic invariants based on the parameter "sym" and then classify these spin configurations into different degeneracy groups such that the configurations in the same group have the same values for all basic invariants (and hence cell potential) and in different groups have at least one different value. We label the degeneracy group in such a way that the ground state configuration, which is the all spin up configuration for ferromagnetic system, belongs to the final group. For each group, we also store the degeneracy D_i (i.e., the number of configurations in the group) and the configurations belonging to this group. We will use $\mathbf{D}$ to denote the vector whose elements are degeneracy, i.e., $\mathbf{D} = (D_1, D_2, \ldots, D_{I+1})$.

3. *Calculation of the column vector* $T^{-1}\mathbf{C}$. In this section, we will derive

[1] This method of generating all possible binary spin configuration was described for the percolation problem in P. J. Reynolds, Ph.D. thesis, MIT, 1979.

formulas for the vector $T^{-1}\mathbf{C}$, which appears at the end of Eqs. (17) and (18). From Eq. (5b), it is easy to show that

$$K_0^{(\alpha)} = \frac{1}{NCF} \sum_{i=1}^{l+1} v_i^{(\alpha)} D_i. \tag{B1}$$

Thus, Eq. (13) may be rewritten as

$$f^{(\alpha)} = -1/z^{\alpha} \left(1/NCF \sum_{i-1}^{l+1} v_i^{(\alpha)} D_i + \ln 2 \right) \tag{B2a}$$

for $T > T_c$ and

$$f^{(\alpha)} = -1/z^{\alpha} (v_{l+1}^{(\alpha)}) \tag{B2b}$$

for $T < T_c$, where $v_{l+1}^{(\alpha)}$ is the ground state cell potential. We now take the first derivative of Eq. (B2) with respect to q. By the chain rule, it is easy to show that

$$\frac{\delta f^{(\alpha)}}{\delta q} = \frac{-\delta \mathfrak{v}^0}{\delta q} \cdot \frac{\delta \mathfrak{v}^{(1)}}{\delta \mathfrak{v}^0} \cdots \frac{\delta \mathfrak{v}^{(m)}}{\delta \mathfrak{v}^{(m-1)}} \cdots \frac{\delta \mathfrak{v}^{(\alpha)}}{\delta \mathfrak{v}^{(\alpha-1)}} 1/z^{\alpha} \mathbf{C}_0, \tag{B3}$$

where

$$\mathbf{C}_0 = (D_1, D_2, \ldots, D_{l+1})/NCF \equiv \mathbf{D}/NCF \tag{B4a}$$

for $T > T_c$ and

$$\mathbf{C}_0 = (0, 0, \ldots, 0, 1) \tag{B4b}$$

for $T < T_c$. Comparing Eqs. (17) and (B3), it is obvious that $T^{-1}\mathbf{C}$ of Eq. (17) is just $\mathbf{C}_0$ of Eq. (B3) and (B4).

ACKNOWLEDGMENTS

We would like to acknowledge useful comments by P. J. Reynolds and the other reviewer of the manuscript.

REFERENCES

1. L. P. KADANOFF, A. HOUGHTON, AND M. C. YALABIK, *J. Statist. Phys.* **14** (1976), 171–203.
2. S. L. KATZ AND J. D. GUNTON, *Phys. Rev. B* **16** (1977), 2163–2167.
3. Y. M. SHIH, *et al.*, *Phys. Rev. B.* **19** (1979), 529–532.
4. M. N. BARBER, *J. Comput. Phys.* **34** (1980), 414–434.
5. C. K. HU, *et al.*, unpublished.
6. Y. M. SHIH, *et al.*, *Phys. Rev. B* **21** (1980), 299–303.
7. M. C. CHANG AND A. HOUGHTON, *Phys. Rev. B.* **21** (1980), 1881–1892.

8. M. C. CHANG AND A. HOUGHTON, *Phys. Rev. Lett.* **44** (1980), 785–788.
9. L. ONSAGER, *Phys. Rev.* **65** (1944), 117.
10. C. N. YANG, *Phys. Rev.* **85** (1952), 808.
11. J. W. ESSAM AND M. E. FISHER, *J. Chem. Phys.* **38** (1963), 802.
12. C. DOMB, *in* "Phase Transitions and Critical Phenomena" (C. Domb and M. S. Green, Eds.), Vol. 3, p. 357, Academic Press, London/New York, 1974.
13. H. E. STANLEY, "Introduction to Phase Transitions and Critical Phenomena," p. 131, Oxford Univ. Press, New York/Oxford, 1971.
14. C. K. HU AND P. KLEBAN, unpublished.
15. M. NAUENBERG AND B. NIENHUIS, *Phys. Rev. Lett.* **33** (1974), 1598–1601.
16. W. VAN SAARLOOS, J. M. J. VAN LEENWEN, AND A. M. M. PRUISKEN, Physica (Netherlands) **92A** (1978), 323–342.
17. M. P. M. DEN NIJS AND H. J. F. KNOPS, *Phys. A* **93A** (1978), 441–456.
18. M. N. BARBER, *J. Phys. A* **10** (1977), 1721.