Calculation of free energies for a three-dimensional Ising model by a modified Kandanoff's variational method

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The modified Kadanoff's variational method recently considered by us is applied to calculate the free energies and their derivatives for a three-dimensional Ising model with bcc structure and without external magnetic field. We find a critical point at $k_c = 0.162\,134$ and the associated critical indices $\alpha = 0.12$, $\alpha' = 0.095$.

I. INTRODUCTION

Although at present, we have very reliable basic principles for microscopic physics at atomic dimensions, we still cannot understand many problems at these dimensions which involve many degrees of freedom. Several efforts have been made to resolve such many-body problems, one of which is the renormalization-group (RG) approach[1] developed in recent years.

In 1976, Kadanoff and co-workers[2] constructed a lower-bound renormalization-group transformation with variational parameters. They applied it to two-, three-, and four-dimensional Ising models and found that the obtained fixed points and critical indices are consistent with exact and series-expansion values. They also wrote down an approximate lower-bound equation for the free energy where the estimation errors become unimportant after many steps (say n) of renormalization-group transformation. At the same time they considered the variation of variational parameters in these n steps of RG transformations to obtain the optimum final free energies. They applied this method to the two-dimensional Ising model and found that the obtained free energies have at most an error of 0.5% as compared with Onsager's exact solution.[3] However the obtained optimum variational parameters in this case differ from the values obtained in the solution of the fixed-point equation. They considered this as an internal contradiction.

In 1977, we[4-6] found that there is no internal contradiction at all in this case. We also considered the variation of variational parameters at each step of the RG transformation; this method will be called the modified Kadanoff's variational method (MKVM). The application of the simplest version of the MKVM to the one-[7] and two-[5] dimensional Ising models with two spin components and without magnetic field is very successful. The MKVM is much simplier than Kadanoff's original method. So this advancement is of real significance.

As a further application of the MKVM, we use it in this paper to calculate the free energies of the three-dimensional Ising model with body-center structure and nearest-neighbor interaction but without external magnetic field. Such problem has no exact solution and is almost untouchable by Kadanoff's original variational method although its

solution is important for the understanding of a realistic system, such as a binary alloy.

The contents, are as follows: In Sec. II, we introduce the calculation procedure used in this paper. In Sec. III, the calculated free energies and their derivatives are presented and plotted. A singlarity at $k_c = 0.162\,134$ is clearly seen, which is near the value, $k_c = 0.157\,40$ obtained by high-temperature series-expansion method.[8] The derivatives of the free energies near singularities are used to obtain the critical indices; we find that $\alpha = 0.12$ and $\alpha' = 0.095$. In Sec IV, we give a brief discussion of our results.

II. CALCULATION METHOD

The Hamiltonian for the three-dimensional Ising model with body-center structure and the nearest-neighbor interaction may be written

$$H = -k \sum_{\langle n,n \rangle} \sigma_i \sigma_j = -\sum_R v_R \ , \qquad (1)$$

$$v_R = k\sigma_9(\sigma_1 + \sigma_2 + \cdots + \sigma_8) \ ,$$

where R is the building block of the lattice with eight spins $(\sigma_1, \sigma_2, \ldots, \sigma_8)$ at the corner and one spin (σ_9) in the center, and the v_R's are the interaction energies within a block. The partition function for the system may be written

$$Z = \sum_{\{\sigma\}} e^{-H} = \sum_{\{\sigma\}} \prod_R e^{v_R} \ . \qquad (2)$$

Summing up all the spin states for the spins in the center of blocks, it is easy to show that Z may be rewritten

$$Z = \sum_{\{\sigma\}} \prod_R e^{v_R^{\text{eff}}} = \sum_{\{\sigma\}}{}' \exp\left(\sum v_R^{\text{eff}} \right) \ , \qquad (3)$$

where

$$v_R^{\text{eff}} = \ln 2 \cosh(k s_1) \ , \qquad (4)$$

$$s_1 = \sigma_1 + \sigma_2 + \cdots + \sigma_8$$

and the summation symbol $\sum'_{\{\sigma\}}$ sums up only the remaining spins in the lattice, i.e., the spins on a simple cubic lattice. At this point, we may regard $-\sum_R v_R^{\text{eff}}$ as the Hamiltonian for a simple cubic lattice. We will use this effective Hamiltonian as the starting point of Kadanoff's lower-bound RG transformation. The new Hamiltonian has the advantage that v_R^{eff} has permutation symmetry with respect to eight spins within the building block and the required calculations in the RG transformation are considerably reduced. This is one of the reasons why we take the body-center cubic as the initial structure. In a future paper, we will consider other lattice structures and symmetry properties of the Hamiltonian, where reduction is also possible by symmetry considerations.

In the one-hypercubic approximation, it is easy to show that the most general Kadanoff's lower-bound renormalization-group transformation[2] for the problem in question may be written

$$e^{v'(\mu)} = \sum_{\sigma_1 \cdots \sigma_8} \exp\left[\frac{p_0}{z} m_1 + p_1 \sum_{i=1}^{8} \mu_i \sigma_i + z v(\sigma) - u(\sigma) \right] \ , \qquad (5)$$

where μ is the spin variable in the new lattice,

$$m_1 = \mu_1 + \mu_2 + \cdots + \mu_8 \ ,$$

$$u(\sigma) = \ln 2(p_0 + p_1 s_1)$$

$$\equiv \ln 2[p_0 + p_1(\sigma_1 + \cdots + \sigma_8)] \ ,$$

p_0, p_1 are variational parameters, and $v(\sigma)$, $v'(\mu)$ are the initial and transformed potential for the basic blocks of the initial and new lattice, respectively.

With the permutation-symmetry v^{eff} of Eq. (4) as the initial potential on the right-hand side of Eq. (5), it is easy to show that $v'(\mu)$ on the left-hand side also has permutation symmetry. To preserve up-down symmetry after the RG transformation of Eq. (5), we must set $p_0 = 0$. The permutation symmetry reduces the 81 configurations of eight spins in the block into nine groups, all configurations of the same group have the same energy before and after the RG transformation and may be changed into each other by a mere permutation transformation. The up-down symmetry reduces the nine groups further to five groups of different energies before and after the RG transformation. For each group of configurations, it is necessary to calculate one transformed potential for a representive configuration on the right-hand side of Eq. (5). The symmetry considerations reduce the calculations considerably. From now on, we will set $p_0 = 0$.

The free energies after the RG transformation are given by

$$F'(H') = -\ln \sum_{\mu_1 \cdots \mu_{N'}} \exp\left(\sum_R v'(\mu) \right) \ ,$$

$$H' = -\sum_R v'(\mu) \ , \qquad (6)$$

where $v'(\mu)$ for an individual block of the new lattice is given by the left-hand side of Eq. (5), and N' is the number of new spins, i.e., $N' = \frac{1}{8}N$. $F'(H')$ is smaller than the original free energies. To determine the optimum variational parameters such that $F'(H')$ approaches the original free energy as close as possi-

ble, we must consider the variation of $F'(H')$ with respect to p_1,

$$\delta F'(H') = -\left[\sum_{\mu_1 \cdots \mu_{N'}} \sum_R \frac{\partial v'}{\partial p_1} \exp\left(\sum_R v'\right) \Big/ \sum_{\mu_1 \cdots \mu_N'} \exp\left(\sum_R v'(\mu)\right)\right] \delta p_1 = 0 \ ,$$

i.e., we must solve the equation

$$\left[\sum_{\mu_1 \cdots N'} \sum_R \frac{\partial v'}{\partial p_1} \exp\left(\sum_{R'} v'\right) \Big/ \sum_{\mu_1 \cdots \mu_N} \exp\left(\sum_R v'\right)\right] = N' \left[\sum_{\mu_1 \cdots \mu_N'} \frac{\partial v'}{\partial p_1} \exp\left(\sum_R v'\right) \Big/ \sum_{\mu_1 \cdots \mu_N'} \exp\left(\sum_{R'} v'\right)\right] = 0 \ . \quad (8)$$

However, to solve Eq. (8) is as difficult as to carry out the configuration sum in the original lattice. Thus we must make some approximations. In the simplest one-block approximation (we call it the one-block approximation of the MKVM), we take only one block in Eq. (8), i.e.,

$$\left[\sum_{\mu_1 \cdots \mu_8} \frac{\partial v'}{\partial p} \exp[v'(\mu_1 \cdots \mu_8)] \Big/ \sum_{\mu_1 \cdots \mu_8} \exp[v'(\mu_1 \cdots \mu_8)]\right] = 0 \ . \quad (9)$$

It has been shown that the one-block approximation of the MKVM is very good for the one-[7] and two-[5]dimensional Ising model without magnetic field (in this case we set $p_0 = 0$ throughout the calculation). Thus we make the same approximation in the case of the three-dimensional Ising model without magnetic field, i.e., we solve Eq. (9) to determine the optimum $p_1 (p_0 = 0$ in this case) for the RG transformation of Eq. (5). Once $v'(\mu)$ is determined for such an optimum p_1, we may use $v'(\mu)$ as the initial potential for the next step of the RG transformation and determine the optimum p_1 in the same way as before.

In the same spirit as in Kandanoff's original paper,[2] we may estimate the free energy per cubic $f^{(\alpha)}$ of the original body-center cubic lattice from the $v^{(\alpha)}(\mu)$ obtained after the α step of the RG transformation. We write it

$$f^{(\alpha)} \simeq \frac{-1}{8^\alpha \times 2} (\ln 2 + \bar{v}^{(\alpha)}) \ , \quad (10)$$

where

$$\bar{v}^{(\alpha)} = \left[\sum_{\mu_1 \cdots \mu_8} v^{(\alpha)}(\mu) \exp[v^{(\alpha)}(\mu)] \Big/ \sum_{\mu_1 \cdots \mu_8} \exp[v^{(\alpha)}(\mu)]\right] \ .$$

TABLE I A. Obtained values of f, $\partial f/\partial k$, $\partial^2 f/\partial k^2$ for $0.1 \leq k \leq 0.2$ and $0.158 \leq k \leq 0.168$.

k	0.10	0.11	0.12	0.13	0.14	0.15	0.16	0.17	0.18	0.19	0.20
f	−0.715	−0.726	−0.727	−0.733	−0.742	−0.751	−0.762	−0.778	−0.800	−0.825	−0.853
$\partial f/\partial k$	−0.493	−0.567	−0.652	−0.748	−0.863	−1.01	−1.22	−1.90	−2.37	−2.71	−2.97
$\partial^2 f/\partial k^2$	−7.04	−7.89	−8.99	−10.5	−12.7	−16.7	−31.2	−57.4	−39.7	−29.2	−22.2

k	0.158	0.159	0.160	0.161	0.162	0.163	0.164	0.165	0.166	0.167	0.168
f	−0.7598	−0.7610	−0.7622	−0.7634	−0.7647	−0.7661	−0.7675	−0.7690	−0.7706	−0.7723	−0.7741
$\partial f/\partial k$	−1.169	−1.195	−1.225	−1.259	−1.303	−1.407	−1.495	−1.574	−1.647	−1.716	−1.781
$\partial^2 f/\partial k^2$	−25.25	−27.69	−31.22	−37.35	−60.36	−94.57	−82.88	−75.80	−70.42	−66.52	−63.25

TABLE I B. Obtained value of f, $\partial f/\partial k$, and $\partial^2 f/\partial k^2$ for $0.1615 \leq k \leq 0.1626$ and $0.162130 \leq k \leq 0.162141$.

k	0.1615	0.1616	0.1617	0.1618	0.1619	0.1620	0.1621	0.1622	0.1623	0.1624	0.1625	0.1626
f	−0.7640	−0.7642	−0.7643	−0.7644	−0.7646	−0.7647	−0.7648	−0.7650	−0.7651	−0.7652	−0.7654	−0.765
$\partial f/\partial k$	−1.279	−1.283	−1.288	−1.293	−1.298	−1.303	−1.310	−1.323	−1.335	−1.347	−1.358	−1.368
$\partial^2 f/\partial k^2$	−43.30	−45.11	−47.32	−50.15	−54.07	−60.36	−76.54	−131.3	−117.8	−111.7	−106.7	−103.1

k	0.162130	0.162131	0.162132	0.162133	0.162134	0.162135	0.162136	0.162137	0.162138	0.162139	0.162140	0.162141
f	−0.76486	−0.76487	−0.76487	−0.76487	−0.76487	−0.76487	−0.76487	−0.76487	−0.76487	−0.76488	−0.76488	−0.76488
$\partial f/\partial k$	−1.3126	−1.3127	−1.3129	−1.3130	−1.3131	−1.3133	−1.3135	−1.3137	−1.3138	−1.3140	−1.3141	−1.3144
$\partial^2 f/\partial k^2$	−103.4	−107.2	−112.4	−121.4	−176.8	−199.2	−186.1	−179.2	−174.8	−170.8	−167.6	−165.0

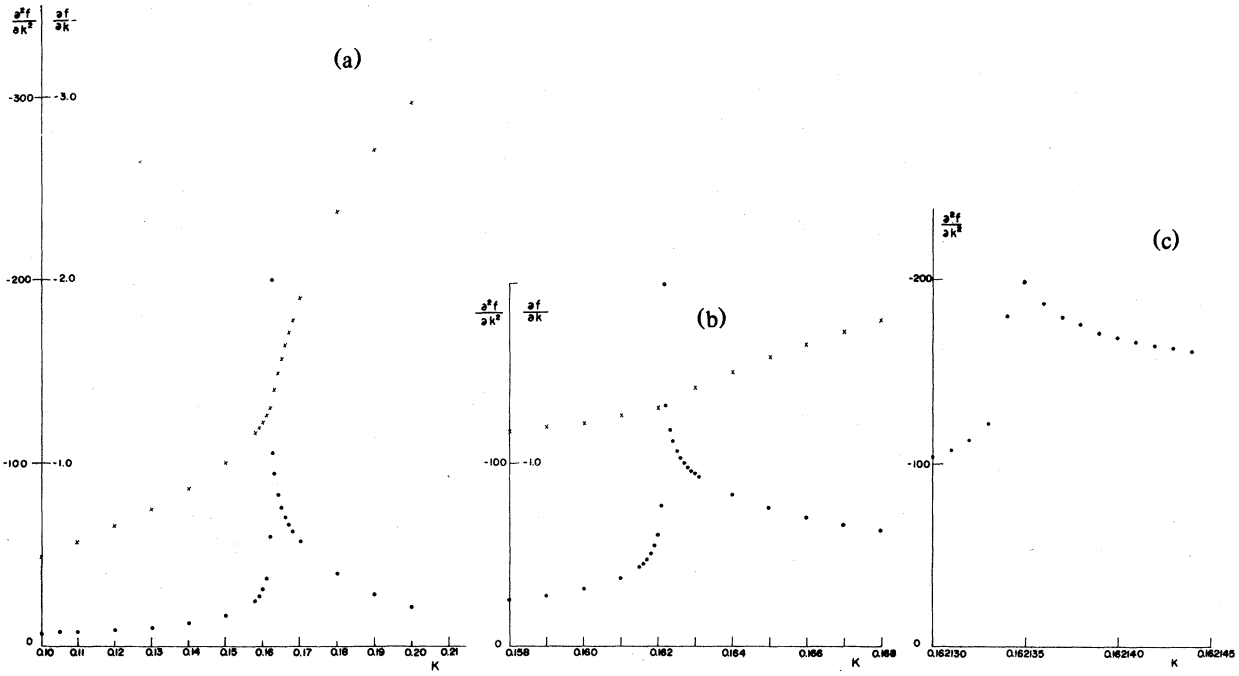

FIG. 1(a) $\partial f/\partial k$ and $\partial^2 f/\partial k^2$ as function of k for $0.10 \leq k \leq 0.20$. The crosses represent $\partial f/\partial k$ and the dots represent $\partial^2 f/\partial k^2$. Inside (outside) scale of vertical axis is for $\partial f/\partial k$ ($\partial^2 f/\partial k^2$). (b) $\partial f/\partial k$ and $\partial^2 f/\partial k^2$ as function of k for $0.158 \leq k \leq 0.168$. The crosses represent $\partial f/\partial k$ and the dots represent $\partial^2 f/\partial k^2$. Inside (outside) scale of vertical axis is for $\partial f/\partial k$ ($\partial^2 f/\partial k^2$). (c) $\partial^2 f/\partial k^2$ as function of k for $0.162130 \leq k \leq 0.162144$.

After many steps of RG transformation, the errors in the estimation of ln2 and $\bar{v}^{(\alpha)}$ are unimportant because in the large α case the contribution of ln2 is small and most of $\bar{v}^{(\alpha)}$ comes from the configuration-independent part of $v^{(\alpha)}(\mu)$, and the estimated $f^{(\alpha)}$ of Eq. (10) will approach a constant value, which is just what we want.

III. FREE ENERGIES AND THEIR DERIVATIVES

We used the CDC 6000 computer with double precision to carry out the numerical calculation. We use subroutine QNWT (modified to double precision) of the Mathematics Science Library to solve Eq. (9) for optimum p_1 and require the left-hand side of Eq. (9) to be less than 10^{-14}. We also require the difference between successive free energies estimated from Eq. (10) in the step-by-step RG transformation to be less than 10^{-15}. To obtain the first and the second derivatives of the free energies with respect to k at a particular k, we calculate the free energies at k and $k \pm \Delta k$ and use the standard differential formula to obtain the result. To check the reliability of the obtained derivatives, we calculate the derivatives at

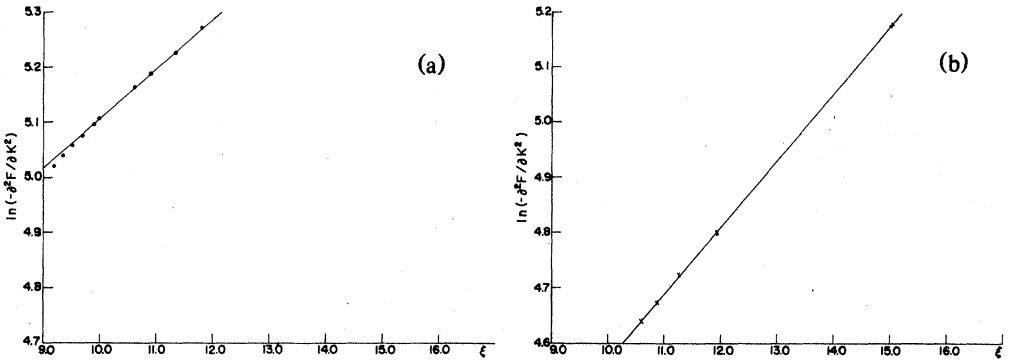

FIG. 2(a) $\ln(-\partial^2 f/\partial k^2)$ as function of $\ln\epsilon$ for $k > k_c$ with $\epsilon = 1 - k_c k$ and $k_c = 0.162\,134\,05$. (b) $\ln(-\partial^2 f/\partial k^2)$ as function of $\ln\epsilon$ for $k < k_c$ with $\epsilon = k_c/k - 1$ and $k_c = 0.162\,134\,05$.

$k = 0.162\,10$ with $\Delta k = 1 \times 10^{-7}$, 5×10^{-7}, and 10×10^{-7}, we find that the difference among the second derivatives is less than 0.14%. We set $\Delta k = 5 \times 10^{-7}$ to calculate the derivatives for other values of k.

The calculated free energies and their first and second derivatives with respect to k are shown in Table I for several ranges of k. We believe that the free energies reported here are the best values one may obtain from Kandanoff and his co-workers lower-bound RG transformation. The first and the second derivatives of the free energy as a function of k are shown in Fig. 1(a)–1(c) for different ranges of k. A singularity around $k = 0.162\,13$ is clearly seen. We have plotted the second derivative of the free energy as a function of $\epsilon = 1 - k_c/k$ for $k > k_c$ and $\epsilon = k_c/k - 1$ for $k < k_c$ on a log scale. We find that as $k_c = 0.162\,134\,05$ the points for $k > k_c$ and $k < k_c$ lie respectively on straight lines. This result is shown on Fig. 2. From the slope of the straight lines we found that $\alpha = 0.12$ and $\alpha' = 0.095$. These values are near the value obtained by the series-expansion method. The k_c we find is also near the value $k_c = 0.15740$ obtained by the series-expansion method.[8]

IV. DISCUSSION

It is well known that in the RG theory of critical indices with the concept of fixed point and linearized RG transformation equation near the fixed point, α' equals to α. The unequality of α and α' in our calculation might be due to the deviation from the RG theory of critical indices or the inaccuracy of our numerical calculation of $\partial^2 f/\partial k^2$ (but not of f itself).

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[1] S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, New York, 1976).
[2] L. P. Kadanoff, A. Houghton, and M. C. Yalabik, J. Stat. Phys. 14, 171 (1976).
[3] L. Onsager, Phys. Rev. 65, 117 (1944).
[4] Y. M. Shih, D. C. Jou, C. K. Pan, W. S. Lee, W. D. Chen, H. M. Huang, C. K. Hu, K. G. Chen, and H. C. Tseng, Chin. J. Phys. 15, 236 (1977).
[5] Y. M. Shih, D. C. Jou, C. K. Pan, W. S. Lee, W. D. Chen, H. M. Huang, C. K. Hu, K. G. Chen, and H. C. Tseng, Phys. Rev. B 19, 529 (1979).
[6] Y. M. Shih, D. C. Jou, C. K. Pan, W. S. Lee, W. D. Chen, H. M. Huang, C. K. Hu, K. G. Chen, and H. C. Tseng, Chin. J. Phys. 16, 181 (1978).
[7] C. K. Hu, S. P. Liu, D. S. Wan, D. C. Jou, C. K. Pan, Y. M. Shih, W. D. Chen, H. M. Huang, K. G. Chen, W. S. Lee, and H. C. Tseng (unpublished).
[8] M. F. Sykes, D. L. Hunter, D. S. McKenzie, and B. R. Heap, J. Phys. A 5, 667 (1972).