Double-chain approximation for the Ising model

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A double-chain approximation for the Ising model is formulated. With the approximation, transition temperatures for several numbers of nearest-neighbor chains are obtained.

I. INTRODUCTION

Cluster methods have been used, and played an important role in the study of critical phenomena for many years.[1] Recently, Suzuki has developed the coherent-anomaly method (CAM),[2] in which cluster methods have been used intensively.[2,3] New cluster methods would also be interesting from such a standpoint.

Here, a double-chain approximation is introduced, in which the solution of the Ising model on a double chain[4] is used. In this approximation, transition temperatures, for example, are easily obtained for an arbitrary number of nearest-neighbor chains z. The square lattice and the cubic lattice correspond to $z=2$ and 4, respectively.

By use of the solution of the Ising model on a double chain, a double-chain approximation is formulated in Sec. II. In Sec. III, some results, including transition temperatures for several z are given, and we mention a critical property applying the CAM to the present approximation.

II. FORMULATION OF THE APPROXIMATION

The double-chain approximation considered here can be thought of as a natural extension of the pair approximation. As a result, a similar formulation is possible.

The free energy per one pair for the double chain in Fig. 1(a) is denoted by $f^{(2)}$ and the free energy per one site for the single chain in Fig. 1(b) is denoted by $f^{(1)}$. In the figure, J and h represent a ferromagnetic coupling and an external field, respectively. Effective fields for the double chain h^{EF} and for the single chain H^{EF} should be determined self-consistently. Both chains are assumed to obey the periodic boundary condition. As the free energy is a function of the magnetization m, with partition functions for the double and single chains denoted by $Z^{(2)}$ and $Z^{(1)}$, respectively, $f^{(2)}$ and $f^{(1)}$ become

$$-\beta f^{(2)}=\lim_{N\to\infty}\frac{\ln Z_N^{(2)}}{N}-2\beta(h+h^{\mathrm{EF}})m\ , \tag{1}$$

$$-\beta f^{(1)}=\lim_{N\to\infty}\frac{\ln Z_N^{(1)}}{N}-\beta(h+H^{\mathrm{EF}})m\ , \tag{2}$$

where N is the length of the chains and we consider the $N\to\infty$ limit. As in the case of the pair approximation, the free energy per one site is given by

$$\beta f(m)=\frac{z}{2}(\beta f^{(2)}-2\beta f^{(1)})+\beta f^{(1)}$$

$$=\frac{z}{2}\beta f^{(2)}+(1-z)\beta f^{(1)}\ , \tag{3}$$

where z is the number of nearest-neighbor chains.

The Ising model considered here is described by the following Hamiltonian:

$$\mathcal{H}=-J\sum_{\langle i,j\rangle}S_iS_j-h\sum_i S_i\ . \tag{4}$$

The sum in the first term is over all nearest-neighbor spins.

First, we consider the single-chain part. The effective Hamiltonian for the single chain corresponding to the Hamiltonian (4) is given by

$$\mathcal{H}^{(1)}=-J\sum_i S_iS_{i+1}-(h+H^{\mathrm{EF}})\sum_i S_i\ . \tag{5}$$

This is just the one-dimensional Ising model in a field. With the notation of $\nu\equiv\beta J$ and $B^{(1)}\equiv\beta(h+H^{\mathrm{EF}})$, $\lim_{N\to\infty}[(\ln Z_N^{(1)})/N]$ becomes

$$\lim_{N\to\infty}\frac{\ln Z_N^{(1)}}{N}=\frac{\sum_{\{S\}}\exp(-\beta\mathcal{H}^{(1)})}{N}=\ln\lambda_1$$

$$=\ln[e^{\nu}\cosh B^{(1)}+(e^{2\nu}\sinh^2 B^{(1)}+e^{-2\nu})^{1/2}]\ , \tag{6}$$

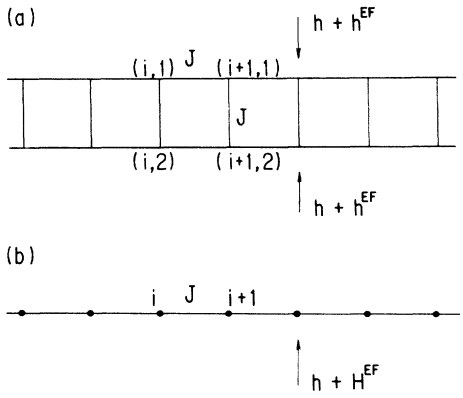

FIG. 1. (a) A double chain and (b) a single chain. A coupling and an external field are denoted by J and h, respectively, and h^{EF} and H^{EF} are effective fields for the double chain and the single chain, respectively.

where λ_1 is the larger eigenvalue for the 2×2 transfer matrix. The relation between the magnetization and $B^{(1)}$ is given by

$$m=\sinh B^{(1)}(\sinh^2 B^{(1)}+e^{-4\nu})^{-1/2} . \tag{7}$$

This can be solved inversely and becomes

$$B^{(1)}=\text{arc sinh}\left[\frac{e^{-2\nu}m}{(1-m^2)^{1/2}}\right] . \tag{8}$$

Next, we consider the double-chain part.[4] The effective Hamiltonian for the double chain is given by

$$\mathcal{H}^{(2)}=-J\sum_i (S_{i,1}S_{i+1,1}+S_{i,2}S_{i+1,2}+S_{i,1}S_{1,2}) -(h+h^{\mathrm{EF}})\sum_i (S_{i,1}+S_{i,2}) . \tag{9}$$

Because this is the Ising model on the double chain in a uniform field, with the maximum eigenvalue for the 4×4 transfer matrix denoted by η_1, $\lim_{N\to\infty}(\ln Z_N^{(2)}/N)$ becomes

$$\lim_{N\to\infty}\frac{\ln Z_N^{(2)}}{N}=\lim_{N\to\infty}\frac{\sum_{\{S\}}\exp(-\beta\mathcal{H}^{(2)})}{N}=\ln\eta_1 . \tag{10}$$

With $B\equiv\beta(h+h^{\mathrm{EF}})$, η_1 is given by

$$\eta_1 2r^{1/3}\cos(\theta/3)+\tfrac{2}{3}(e^{2\nu}\cosh2B+e^{-\nu}\cosh2\nu) . \tag{11}$$

In this expression, r and θ are given by

$$r^{1/3}=\tfrac{2}{3}[(e^{-\nu}\cosh2\nu+e^{3\nu}\cosh2B)^2 -3e^{2\nu}\sinh2\nu(\cosh2B+\cosh2\nu)]^{1/2} , \tag{12}$$

and

$$\theta=\text{arc tan}\frac{(-q^2-4p^3)^{1/2}}{-q}+\pi\Theta_H\left[\frac{(-q^2-4p^3)^{1/2}}{q}\right] , \tag{13}$$

where $\Theta_H(x)$ is the Heaviside's step function and p and q are expressed by ν and B as follows:

$$p=\tfrac{4}{9}[3e^{2\nu}\sinh2\nu(\cosh2B+\cosh2\nu)-e^{-\nu}\cosh2\nu+e^{3\nu}\cosh2B)^2] ,$$
$$q=\tfrac{8}{27}[-2(e^{-\nu}\cosh2\nu+e^{3\nu}\cosh2B)^3+9e^{2\nu}\sinh2\nu(e^{-\nu}\cosh2\nu+e^{3\nu}\cosh2B)(\cosh2B+\cosh2\nu)-27e^{\nu}\sinh^2 2\nu] . \tag{14}$$

The magnetization is given by

$$m=\frac{1}{\eta_1}\left\{\frac{1}{3}r^{-5/3}\left[\frac{\partial r^2}{\partial(2B)}\cos(\theta/3) -\tfrac{1}{4}\sin(\theta/3)\left[\frac{q}{(-q^2-4p^3)^{1/2}}\frac{\partial(q^2+4p^3)}{\partial(2B)}+2(-q^2-4p^3)^{1/2}\frac{\partial q}{\partial(2B)}\right]\right]+\tfrac{2}{3}e^{3\nu}\sinh2B\right\} . \tag{15}$$

Unlike the single-chain case, it seems difficult to solve it inversely.

Using (1), (2), (3), (6), and (10), the free energy is rewritten as follows:

$$\beta f(m)=\frac{z}{2}(-\ln\eta_1+2Bm)+(1-z)(-\ln\lambda_1+B^{(1)}m) . \tag{16}$$

The magnetization can be obtained by solving the following equation:

$$\frac{\partial f(m)}{\partial m}=h . \tag{17}$$

In the case of $h=0$, (17) becomes

$$\frac{z}{2}(2B)+(1-z)B^{(1)}=0 . \tag{18}$$

As noted earlier, it is difficult to express B as a function of m. The magnetization is obtained by solving (18) numerically. Among solutions, the real magnetization minimizes the free energy (16), which can be proved from a thermodynamic inequality and (17).

III. RESULTS

Magnetizations for arbitrary z can be obtained from (16) and (18). As an example magnetizations for $z=2$ (square lattice) and $z=4$ (cubic lattice) are shown in Fig. 2.

Transition temperatures can be obtained by solving (18) directly or more simply by seeking the zero point of the coefficient of the first-order term in m when the left-

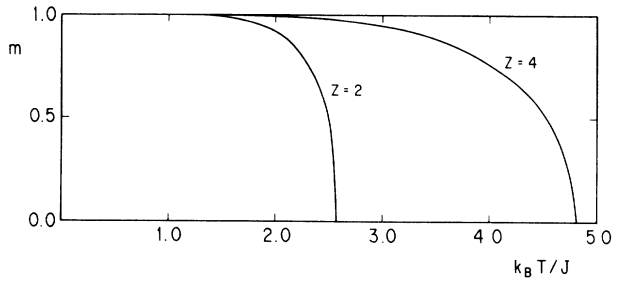

FIG. 2. Magnetizations for $z=2$ (square lattice) and $z=4$ (cubic lattice) in the double-chain approximation.

hand side of (18) is evaluated in terms of m. The latter method can be applied when the transition is second order as in the present case. In (18), $B^{(1)}$ can be evaluated easily in terms of m using (8), and it is also a simple task to evaluate B by using (15). The transition temperatures T_c for $z=2$, 3, 4, and 6 are given in Table I, together with the exact value for $z=2$ and a Monte Carlo renormalization group result for $z=4$.[5] In the table, critical coefficients of the susceptibility, which will be explained later, are also shown.

Next, we mention an application of the double-chain approximation to estimate the susceptibility exponent γ by means of the CAM theory.[2] In the CAM theory, at least two cluster approximations are needed to calculate critical exponents. Here we use the double- and single-chain approximations to estimate the critical exponent of the susceptibility.

In a cluster approximation, the susceptibility $\chi_0(T)$ near the critical point and its critical coefficients $\bar{\chi}$ are related by the following equation:[2]

$$\chi_0(T)\simeq\frac{\bar{\chi}}{\varepsilon},\quad \varepsilon=\frac{T-T_c}{T_c}\ . \tag{19}$$

Critical coefficients of the susceptibility for $z=2$, 3, 4, and 6 in the double-chain approximation are given in Table I. We need another approximation to apply the CAM. In the single-chain approximation, the transition temperature $T_c^{(1)}$, and the critical coefficient $\bar{\chi}^{(1)}$ are obtained from the following equation:

$$z\frac{J}{k_BT_c^{(1)}}\exp(2J/k_BT_c^{(1)})=1 \tag{20}$$

and

$$\bar{\chi}^{(1)}=\frac{1}{zJ(2J/k_BT_c^{(1)}+1)}\ . \tag{21}$$

The critical exponent γ is estimated by[2]

TABLE I. Transition temperatures T_c in the double-chain approximation for $z=2$, 3, 4 and 6 and the real values T_c^* for $z=2$ and 4. Critical coefficients of the susceptibility $\bar{\chi}$ in the double-chain approximation, which are defined by (19), are also given.

z	k_BT_c/J	$k_BT_c^*/J$[a]	$\bar{\chi}J$
2	2.575 88	2.269 18...	0.826 56
3	3.739 54		0.404 21
4	4.815 77	4.511 53...	0.275 90
6	6.888 39		0.173 00

[a]Reference 5.

$$\gamma-1\simeq\frac{\ln(\bar{\chi}^{(1)}/\bar{\chi})}{\ln[(T_c-T_c^*)/(T_c^{(1)}-T_c^*)]}\ , \tag{22}$$

where T_c^* is the real transition temperature.[5] From (22), we obtain $\gamma\simeq1.675$ and 1.296 for the square ($z=2$) and the cubic ($z=4$) lattices, respectively. These results are not so bad, although only the first two cluster approximations are used in a series of approximations. The two approximations may be thought of as a part of a canonical series of approximations in the CAM theory.

In conclusion, we have studied the Ising model for an arbitrary number of nearest-neighbor chains in terms of the double-chain approximation which can be treated numerically. This approximation is an extension of the pair approximation, which is equivalent to the Bethe approximation,[6] and at the same time, an extension of the single-chain approximation. Transition temperatures and magnetizations have been obtained, and these values are closer to the real values than those obtained by the pair and single-chain approximations. This is a natural consequence because more fluctuations are included in the present approximation.

[1]See, e.g., J. M. Ziman, *Models of Disorder* (Cambridge University Press, Cambridge, England, 1979), Sec. 5.4.
[2]M. Suzuki, J. Phys. Soc. Jpn. **55**, 4205 (1986).
[3]M. Suzuki, M. Katori, and X. Hu, J. Phys. Soc. Jpn. **56**, 3092 (1987); M. Katori and M. Suzuki, *ibid.* **56**, 3113 (1987).
[4]T. Yokota (unpublished).
[5]We use the exact result of L. Onsager [Phys. Rev. **65**, 117 (1944)] for $z=2$ and the result of G. S. Pawley, R. H. Sweden, D. J. Wallace, and K. G. Wilson [Phys. Rev. B **29**, 4030 (1984)] for $z=4$.
[6]H. A. Bethe, Proc. R. Soc. London, Ser. A **150**, 552 (1935).