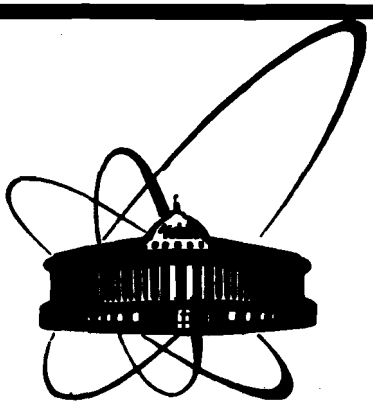

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A TRANSFER-MATRIX CLUSTER APPROXIMATION FOR LATTICE MODELS

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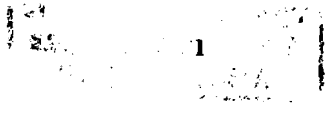
I. INTRODUCTION

There are two important classical approaches to calculation of the free energy, correlation functions and other thermodynamic properties of lattice models with discontinuous site variables: cluster variation methods (CVM)[1,2,3] and the transfer-matrix method[4]. In the first one, the free energy is constructed from the configuration probabilities of a finite cluster, and to obtain thermodynamic quantities, it is minimized with respect to unknown probabilities. The cluster variation methods yield explicitly low symmetry phases and phase transitions between them and the high symmetry phase varying the temperature or other parameters. They give classical critical exponents but renormalization group ideas are easily applied to them[5]. However, it is not clear how to construct the free energy functional in the most effective way and the minimization procedure is generally tedious for higher approximations and long-range interactions.

The transfer matrix method is applicable only to one - dimensional systems and instead of higher-dimensional systems only one-dimensional slabs or strips are in fact treated by it. Naturally, for these systems no phase transitions occur. Nevertheless, the values of critical temperature and critical exponents can be derived from a finite-size scaling procedure[6] but no values of the low symmetry correlation functions are available. The simplicity of mathematical methods being used allows one to treat large systems with rather long range interactions[7].

Our treatment combines both the mathematical simplicity of T-matrix method and the explicit occurrence of low symmetry phases and phase transitions of CVM's. The construction of an arbitrary approximation is straightforward and the method is more effective than CVM as it uses less unknown parameters than is the number of configuration probabilities in CVM of the same accuracy. The results are obtained by simple iterations.

Recently, there has appeared a double-chain approximation for the Ising model[8] similar, to some extent, to our approach. But our method, in



distinction to it, is applicable to very general lattice models, uses a number of multi-site mean fields instead of a one single-site field, and can be formulated with arbitrary accuracy.

To solve the two-dimensional Ising model, Suzuki et al.[9,10] used one-dimensional strips with a single-site mean field at the boundaries. From the point of view of that paper our method may be considered as a one reducing the two-dimensional problem to a strip with multi-site mean fields now applied only to a one boundary.

The method is formulated in Sec. II and the example of Ising model in Sec. III is used to illustrate it. The accuracy of the approximate values of the critical temperature is within 0.1% for comparatively low approximations, what is a better result than in[8,9].

II. METHOD

We shall develop an approximate method for calculation of the correlation functions and the free energy of two-dimensional lattice models with discontinuous site variables described by the Hamiltonian

$$H = \sum_{i=1}^{M} H_i(\{K_i\};\ n_{i_1},\ldots,n_{i_j}), \qquad (1)$$

where i numbers lattice sites, n_{i_k} are site variables at sites in a finite size area around the site i. $n_i = 0,1,\ldots,N$ (in the illustrative calculations below for the Ising model, we put $N = 1$). If the interaction constants K_i's are of finite range the site Hamiltonians H_i may be written explicitly in the following form

$$H_i(\{K_i\};n_{i_1},\ldots,n_{i_j}) = \sum_{m_{i_1},\ldots,m_{i_j}} K(m_{i_1},\ldots,m_{i_j})\,\delta(m_{i_1},n_{i_1})\ldots\delta(m_{i_j},n_{i_j}), \qquad (2)$$

where j is the number of the lattice sites in the cluster around the site i. Its diameter is given by the largest interaction range; (2) is the most general form of a classical Hamiltonian with finite range interactions.

For calculation of the partition function $Z = \sum_{\{n_i\}} \exp(H(n_i))$ (the factor $-1/k_BT$ is absorbed in the interaction constants), it is useful

to introduce a transfer matrix T_i defined by the relation

$$\exp(H(n_i)) = \prod_{i=1}^{M} T_i(N_i,N_{i+1},\ldots,N_{i+k});$$

i numbers the rows of the lattice and $M\to\infty$ is the number of the rows in the whole lattice; $N_j = \{n_{j,k}\}$ is the set of the lattice site variables in the j-th row, and k is at least as large as the range of interactions perpendicular to the rows. For homogeneous lattices we take all T_j in the same form. The above definition of T-matrix is not unambiguous and yields a lot of freedom how to choose it. We impose only two limitations on the choice of the T-matrix: the T-matrix (together with the Hamiltonian) should be invariant with respect to transformations corresponding to the symmetry which we expect to be broken for some values of interaction parameters, and for the sake of simplicity, it should be as small as possible. The T-matrix can obviously be written in the exponential form, as well

$T_i(N_i,N_{i+1},\ldots,N_{i+k}) = \exp(G_i(\{K_i\};N_i,N_{i+1},\ldots,N_{i+k}))$,
where $\sum G_i = H$.

As is well known, the free energy of the system and the correlation functions are directly related to the largest eigenvalue and to the corresponding eigenvector of the equation

$$\sum_{N_{i+k}} T_i(N_i,N_{i+1},\ldots,N_{i+k})\Psi_i(N_{i+1},\ldots,N_{i+k}) = \lambda_i\Psi_i(N_i,\ldots,N_{i+k-1}). \qquad (3)$$

Generally, it is not possible to solve this equation exactly as the T-matrix as well as the eigenvector are infinite along the rows. Usually, this problem is treated by solving the problem for a strip of a finite width with appropriate boundary conditions. Then, the problem turns out to be effectively one - dimensional and no phase transitions nor spontaneous symmetry breaking appears. In our approach we leave both T-matrix and the eigenvector infinite, but we approximate the eigenvector by a finite number of parameters L_i and J_i

$$\Psi_i(N_{i+1},\ldots,N_{i+K}) = \sum_{N_{i+k+1},\ldots,N_{i+k+t}} \exp\Big(g_{i+1}(\{L_p\};N_{i+1},\ldots,N_{i+k}) + h_{i+1}(\{J_r\};N_{i+1},\ldots,N_{i+k},N_{i+k+1},\ldots,N_{i+k+t})\Big). \qquad (4)$$

Substituting (3) into (2) we get

$$\sum_{N_{i+k}} \sum_{N_{i+k+1},\ldots,N_{i+k+l}} \exp\Big(G_i(\{K_i\};N_1,\ldots,N_{i+k}) + g_{i+1}(\{L_p\};N_{i+1},\ldots,N_{i+k}) + h_{i+1}(\{J_r\};N_{i+1},\ldots,N_{i+k},N_{i+k+1},\ldots,N_{i+k+l})\Big) =$$

$$= \lambda_i \sum_{N_{i+k},\ldots,N_{i+k+l-1}} \exp\Big(g_i(\{L_p\};N_1,\ldots,N_{i+k-1}) + h_i(\{J_r\};N_1,\ldots,N_{i+k-1},N_{i+k},\ldots,N_{i+k+l-1})\Big) . \qquad (5)$$

We assume that both g_i and h_i can be written in the same way as (2), i.e. all the constants L_j and J_j are of a short range character. This assumption represents the only approximation in our method. If we put $h_i = 0$ we obtain a generalized mean field approximation. Instead of a single side mean field, as usually, a set of many-body fields on many-body interactions is included in g_i which is added to the row Hamiltinian G_i. The exact expression for Ψ_i would contain an infinite number of interaction constants L_i and it would exactly represent the influence of one of the half lattices on the other. The many-body interactions generated by g_i in the rows $i+1,\ldots,i+k$ are in fact indirect interactions induced by the lattice variables in the rows $n>i+k$ over which we have already summed up. As the exponentials at the left hand-side of (4) are positive, we see that (4) is valid only for the eigenvector corresponding to the largest eigenvalue.

In our approximate expression g_i, there are no long range interactions that the exact solution does contain. To some extent, they can be simulated by a "mean" lattice represented by the rows $i+k+1,\ldots,i+k+l$ included in h_{i+1} that does not occur in the T-matrix. Nevertheless, the effect of the few extra rows cannot be equivalent to that of the whole infinite half lattice. Really, the decay of pair correlations at the left hand side of eq. (5) is always smaller than the decay of those at its right hand side.

A similar effect as the extra rows added to the left-hand side of the eigenvector is obtained if the rows are added to the right-hand side of both the T-matrix and the eigenvector. In this case, (5) remains unchanged, only h_i is equal to zero and k is larger than the minimum allowed value. Both these modifications improve the results, namely the values of the critical interaction constants.

The vector equation (5) represents an infinite number of nonlinear equations for a finite number of parameters. To obtain the equal number of equations and interaction constants in Ψ_i, we sum up over most of the site variables leaving only such a number of equation as is the number of parameters. It is an easy task to perform the summation because the exponents at both sites of (5) can be considered as (unnormalized) configuration probabilities of infinite one - dimensional strips. Performing the summation (e.g by the T-matrix method), we get what are the configuration probabilities of a finite cluster for the corresponding one-dimensional statistical system. The size of the cluster is given by the requirement that the number of its configurations is equal to the number of parameters L_i and J_i. Then, we have to solve the following equations

$$P_k(\{L_i\},\{J_i\};n_1,\ldots,n_m) = P_{k-1}(\{L_i\},\{J_i\};n_1,\ldots,n_m) \qquad (6)$$

for all configurations of the lattice variables n_i of the cluster. P_k are the configuration probabilities of the given cluster for the k-row statistical system described by the Hamiltonian $H_k = \sum_i (G_i + g_i + h_i)$, while P_{k-1} are the same probabilities for a $(k-1)$-row system with the Hamiltonian $H_{k-1} = \sum_i (g_i + h_i)$. Both probabilities are normalized to unity. If we sum up over all variables at both sides of (5) we get an expression for λ_i i.e. for the free energy

$$\lambda_i = Z_k(G_i,g_i,h_i) / Z_{k-1}(g_i,h_i) , \qquad (7)$$

where Z_k and Z_{k-1} are the partition functions of k-row and $(k-1)$-row systems.

The order of the approximation is given by the number of parameters L_i and J_i, i.e. by the number of sites in the cluster.

The probabilities P_k and P_{k-1} are not the configuration probabilities of our problem described by the Hamiltonian H. These can also be calculated from one-dimensional strips but using the Hamiltonians

$$G(N_1,\ldots,N_{i+k}) + g(N_{i+1},\ldots,N_{i+k}) + g(N_{i+k-1},\ldots,N_1) + h(N_{i+1},\ldots,N_{i+k},N_{i+k+1},\ldots,N_{i+k+l}) + h(N_{i+k-1},\ldots,N_1,N_{i-1},\ldots,N_{i-l}),$$

or

$$g(N_1,\ldots,N_{1+k-1}) + g(N_{1+k-1},\ldots,N_1) + h(N_1,\ldots,N_{1+k-1},N_{1+k},\ldots N_{1+k+1-1})$$

$$h(N_{1+k-1},\ldots,N_1,N_{1-1},\ldots,N_{1-1}).$$

A convenient way how to solve (7) is to use the iteration method which reminds the power method for solving the matrix eigenvalue problem. With the values of interaction constants L_1 and J_1, we calculate the right-hand side of the equation by the T- matrix method and then the interaction constants of the next iteration step from its left-hand side. The latter problem is generally not a simple one, but in some cases it can be solved by straightforward calculations. If h_1 is equal to zero and g_1 has the following explicit form:

$$g_{1+1} = \sum_j g_{1+1,j}\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}$$

$$g_{1+1,j} = \sum_{(m)} L\begin{pmatrix} m_{1+1,j},\ldots,m_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ m_{1+k,j},\ldots,m_{1+k,j+s_{1+k}} \end{pmatrix} \cdot \delta(m_{1+1,j},n_{1+1,j})\ldots\delta(m_{1+k,j+s_{1+k}},n_{1+k,j+s_{1+k}})$$

the free energy of the $(k\text{-}1)$-row strip is the following:

$$F = \sum_{(n)} L\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix} P\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}$$

$$+\sum_{(n)} P\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix} \ln\left(P\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}\right) \qquad (8)$$

$$-\sum_{(n)} P\begin{pmatrix} n_{1+1,j+1},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j+1},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix} \ln\left(P\begin{pmatrix} n_{1+1,j+1},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j+1},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}\right).$$

The meaning of notation in the expression for $g_{1,j}$ is analogous to that in (2). P's are the probabilities of cluster configurations in a $(k\text{-}1)$-row strip and the probabilities in the last row of (8) are obtained from them by summation over the first column; s_1 characterizes the range of the induced interactions J_k along the i-th row. Minimizing the free energy with respect to P's, we get the formula for calculation of interaction constants from configuration probabilities

$$L\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix} = -\ln\left(P\begin{pmatrix} n_{1+1,j},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}\right) + \ln\left(P\begin{pmatrix} n_{1+1,j+1},\ldots,n_{1+1,j+s_1} \\ \vdots \quad\quad \vdots \\ n_{1+k,j+1},\ldots,n_{1+k,j+s_{1+k}} \end{pmatrix}\right). \qquad (9)$$

There is no such a simple formula for calculation of the constants J_1 and L_1 when h_1 is nonzero, because of long range interactions introduced by summation over the rows $i+k+1,..,i+k+l$. To avoid this difficulty, we try to solve a larger set of equations instead of (5)

$$\sum_{N_{1,k}} \exp\Big(G_1(\{K_1\};N_1,\ldots,N_{1+k}) + g_{1+1}(\{L_p\};N_{1+1},\ldots,N_{1+k}) + h_{1+1}(\{J_r\};N_{1+1},\ldots,N_{1+k},N_{1+k+1},\ldots,N_{1+k+1})\Big) =$$

$$= \lambda_1 \exp\Big(g_1(\{L_p\};N_1,\ldots,N_{1+k-1}) + h_1(\{J_r\};N_1,\ldots,N_{1+k-1},\ldots,N_{1+k+1-1})\Big). \qquad (10)$$

Now, if we reduce by summation the whole strip to a cluster of the same width as that of the strip i.e. $(k+1\text{-}1)$, we can repeat the whole above described procedure.

From computational reasons, it is convenient, solving eq. (6), to use compact clusters of the width of the strip at the left-hand side of eq. (3). But in principle, the cluster in (6) may be chosen arbitrary even with sites far apart from each other. In such a way we can change the type of approximation.

An important area of application of the presented method is calculation of phase diagrams in systems with superstructures appearing in various two-dimensional systems, e.g., surface adsorbate and CuO layers in high

temperature superconductors. Now, the symmetry breaking in the problem with a homogeneous Hamiltonian again naturally appears causing all the parameters L_1, J_1 site dependent. They would be periodic functions of the position with a period equal to the period of the superstructure. Then, applying the iteration method to (6) and the power method to the one-dimensional strips, we have to expect the repetition of the iteration procedure only after the number of steps which is equal to the period of the superstructure. As we impose no restriction on the periodicity of the structure in the direction perpendicular to the strips, the method is a powerful tool for studying incommensurate structures.

III. RESULTS FOR THE ISING MODEL

To compare the results of our approximate method with exact solutions, we calculate the critical temperature and magnetization of the two-dimensional Ising model, or two-dimensional lattice gas model on the square lattice with nearest neighbour interactions described by the site Hamiltonian

$$H_{i,j} = K\, n_{i,j}(n_{i,j+1} + n_{i+1,j}) + \mu\, n_{i,j} \qquad (11)$$

$$H = \sum_{i,j} H_{i,j}$$

$$n_{i,j} = 0, 1.$$

We have calculated the free energy, the correlation functions, and the critical temperature for different approximations according to the following choices of the functions $G_i=\sum_j G_{i,j}$, $g_i=\sum_j g_{i,j}$, and $h_i=\sum_j h_{i,j}$:

i) $G_{i,j} = K/2\,(n_{i,j}+n_{i+1,j+1})(n_{i+1,j}+n_{i,j+1}) + \mu/4\,(n_{i,j}+n_{i+1,j}+n_{i,j+1}+n_{i+1,j+1})$

$g_{i,j} = L_1/3\,(n_{i,j}+n_{i,j+1}+n_{i,j+2}) + L_2/2\, n_{i,j+1}(n_{i,j}+n_{i,j+2}) + L_3\, n_{i,j}n_{i,j+2} + L_4\, n_{i,j}n_{i,j+1}n_{i,j+2}$

$h_{i,j} = 0$,

which is a three-site approximation.

ii) $G_{i,j}$ and $h_{i,j}$ are the same as in (i), and

$g_{i,j} = L_1/4\,(n_{i,j}+n_{i,j+1}+n_{i,j+2}+n_{i,j+3}) + L_2/3(n_{i,j+1}(n_{i,j}+n_{i,j+2})+ n_{i,j+2}n_{i,j+3}) + L_3/2\,(n_{i,j}n_{i,j+2} + n_{i,j+1}n_{i,j+3}) + L_4\, n_{i,j}n_{i,j+3} + L_5/2\, n_{i,j+1}n_{i,j+2}(n_{i,j}+n_{i,j+3}) + L_6/2\, n_{i,j}n_{i,j+3}(n_{i,j+1}+n_{i,j+2}) + L_7\, n_{i,j}n_{i,j+1}n_{i,j+2}n_{i,j+3}$

i.e. (ii) is a four-site approximation.

In the case when $h_{i,j}= 0$, the T-matrix for calculation along the strip $t_{i,j} = \exp(G_{i,j} + g_{i+1,j})$ is the same as for a single chain except two sites in the second row originating from $G_{i,j}$.

iii) $G_{i,j}$ is the same as in i) and

$g_{i,j} + h_{i,j} = L_1/2\,(n_{i,j}+n_{i,j+1}) + L_2/2\,(n_{i+1,j}+n_{i+1,j+1}) + L_3/2(n_{i,j}n_{i+1,j}+n_{i,j+1}n_{i+1,j+1}) + L_4\, n_{i,j}n_{i,j+1} + L_5\, n_{i+1,j}n_{i+1,j+1} + L_6\,(n_{i,j}n_{i+1,j+1}+n_{i+1,j}n_{i,j+1}) + L_7\, n_{i,j}n_{i,j+1}(n_{i+1,j}+n_{i+1,j+1}) + L_8\, n_{i+1,j}n_{i+1,j+1}(n_{i,j}+n_{i,j+1}) + L_9\, n_{i,j}n_{i,j+1}n_{i+1,j}n_{i+1,j+1}$

iv) $G_{i,j} = -(7/12)K\,(n_{i,j}+n_{i,j+1}+n_{i+2,j}+n_{i+2,j+1}) + (\mu -(7/6)K)\times(n_{i+1,j}+n_{i+1,j+1}) + K/3\,(n_{i,j}n_{i,j+1}+n_{i+1,j}n_{i+1,j+1}+n_{i+2,j}n_{i+2,j+1}) + K/4\,(n_{i+1,j}(n_{i,j}+n_{i+2,j}) + n_{i+1,j+1}(n_{i,j+1}+n_{i+2,j+2})$

$h_{i,j} = 0$

$g_{i,j}$ is equal to the same expression as $g_{i,j} + h_{i,j}$ in (iii).

The concrete choice of the chemical potential at the edges and in the middle of the strip in (iv) is due to the requirement of invariance of $T_i=\exp(G_i)$ with respect to particle - hole symmetry when $\mu=-2K$ (i.e. magnetic field is equal to zero for the corresponding Ising model).

The values of critical temperature (critical pair interaction $K_c= J/k_BT_c$) for the approximations (i-iv) together with the exact value are given in Tab. 1.

TABLE I

$K_{c,i}$	$K_{c,ii}$	$K_{c,iii}$	$K_{c,iv}$	$K_{c,exact}$
1.775	1.7672	1.7652	1.7638	1.7627

We see that even the lowest approximations give the values of K_c very close to the exact value and the approximations using extra rows (iii, iv) yield better results than (i) and (ii). In our method, working with infinite T-matrices, for $\mu=-2K$ and $K>K_c$ the coverage $\langle n \rangle$ is different from 1/2 (magnetization is nonzero). As our method is of mean field type with the critical exponent of magnetization $\beta=1/2$ instead of the real value 1/8, we cannot expect good coincidence of our coverage curves with the exact one near the phase transition point. The coverage calculated from the approximations (ii) and (iv) and the exact coverage curve is shown in Fig. 1. The values of coverage for the approximation (iii) lie between the curve 2 and 3. From Fig. 1 we see that, if shifted to the exact value of K_c, the approximation (ii) yields better values for coverage than (iv). The method makes it possible to calculate all correlation functions, but again near the phase transition point, we have to expect the decay of long range correlations to be too fast.

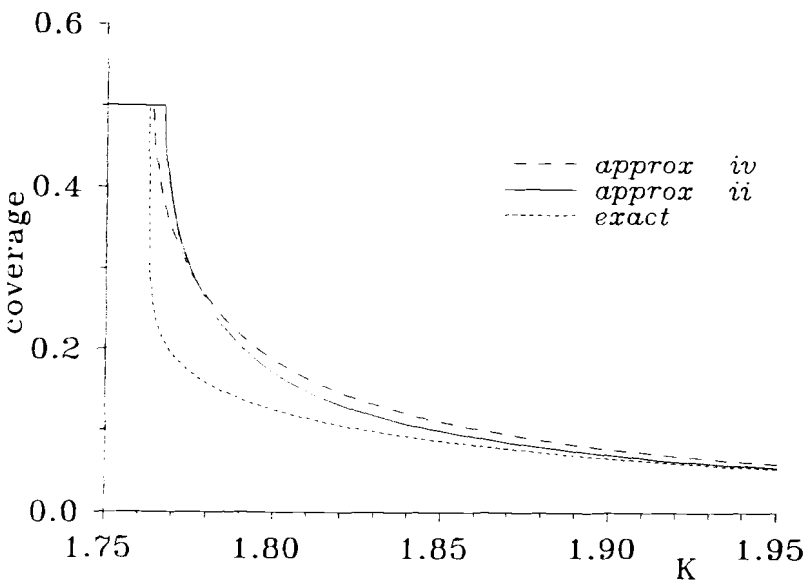


Fig. 1 Coverage as a function of the nearest-neighbour interaction K for $\mu=-2K$; 1- exact result, 2- approximation (iv), 3- approximation (ii). The coverage for the approximation (iii) lies between the curves 2 and 3.

In conclusion, we have developed an approximate method for calculation of thermodynamical properties of a wide class of lattice models of statistical mechanics. The approximation is an extension of the cluster variation methods and the transfer-matrix method. As is shown for the Ising model, the results of the method are very close to the results of the exact solution even in the low order approximations. The order of approximation can be systematically improved in a straightforward way. The symmetry of the results may be lower than the symmetry of the Hamiltonian. The method is a mean-field type approximation but the finite-size scaling and the coherent anomaly method may be applied to it easily. The three-dimensional problems are solved by reducing the dimension of the system at first to two, and in the next step to one dimension.

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