IC/90/253

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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INTERNATIONAL ATOMIC ENERGY AGENCY

UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

1990 MIRAMARE - TRIESTE

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International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization
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A CLUSTER APPROXIMATION FOR THE TRANSFER–MATRIX METHOD *

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ABSTRACT

A cluster approximation for the transfer–method is formulated. The calculation of the partition function of lattice models is transformed to a nonlinear mapping problem. The method yields the free energy, correlation functions and the phase diagrams for a large class of lattice models. The high accuracy of the method is exemplified by the calculation of the critical temperature of the Ising model.

MIRAMARE – TRIESTE
August 1990

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* Submitted for publication.

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I. INTRODUCTION

There are two important classical approaches to the 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. To obtain thermodynamic quantities, the free energy is minimized with respect to unknown probabilities. The cluster-variation methods yield explicitly phases with lower symmetry when compared with the symmetry of the Hamiltonian, phase transitions between them and the high-symmetry phase when the temperature or other parameters are changed. They give classical critical exponents but renormalization-group ideas are easily applied to them.[5] However, it is not clear how to construct, in the most effective way, the free-energy functional. For higher approximations and long-range interactions the minimization procedure is generally tedious.

The transfer matrix method is applicable only to one - dimensional systems. In fact, instead of higher-dimensional systems only one-dimensional slabs or strips are treated by it. Naturally, for these systems no phase transitions occur and all the values of the order parameters of continuous phase transitions are equal to zero. Nevertheless, the values of the critical temperature, the critical exponents and indirectly also the values of order parameters can be derived from a finite-size scaling procedure.[8] The simplicity of mathematical methods allows one to treat large systems with rather long-range interactions.[9]

Our treatment combines both the mathematical simplicity of the T-matrix method and the explicit occurrence of non-zero order parameters 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 the number of unknown configuration probabilities in CVM of the same accuracy. The results are obtained by simple iterations.

The presented method is closely related to the variational approach by Baxter[8] which was later applied to the Ising model by Tsang[9].This relation is discussed in Sections II and III.

Recently, there has appeared a double-chain approximation for the Ising model,[10] 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 one single-site field, and can be formulated with arbitrary accuracy.

To solve the two-dimensional Ising model, Suzuki et al.[11,12] 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 similar problem on a strip with multi-site mean fields applied only to one boundary.

The method is formulated in Sec.II and the example of the 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-order approximations, that is a better result than the values of the critical temperatures in the papers.[9,10,11]

II. METHOD

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

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

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). A set of short-range interaction constants is denoted by $\{K_l\}$. The site Hamiltonians H_i may be written explicitly in the following form

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

where j is the number of the lattice sites of the cluster in the neighborhood of the site i, $K(m_{i_1}, \ldots, m_{i_j})$ is the energy of the cluster configuration $(m_{i_1}, \ldots, m_{i_j})$; $m_k = 0,1,\ldots,N$. The diameter of the cluster is given by the range of the interactions. The expression (2) is the most general form of a classical lattice Hamiltonian with finite range interactions. (In the case of the Ising-type lattice gas model with nearest-neighbor interactions on the square lattice, the values of the parameters in (2) may be chosen as follows: j=3, $i = i_2 \equiv (l,k)$, $i_1 \equiv (l+1,k)$, $i_3 \equiv (l,k+1)$, $K(1,1,1) = 2K + \mu$, $K(0,1,1) = K(1,1,0) = K + \mu$, $K(0,1,0) = \mu$, $K(m_{i_1}, 0, m_{i_3}) = 0$, where K is the nearest-neighbor pair interaction and μ is the chemical potential (cf.Eq.(11)). Other possible choices of the clusters

are depicted in Fig.1 by squares with vertical bars.)

For the calculation of the partition function $Z = \sum_{\{n_i\}} \exp(H(n_i))$ (the factor $-1/k_B T$ 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; $N_i = \{n_{i,j}\}$ is the set of the lattice site variables in the j-th row, and the width of the strip k is at least as large as the range of interactions perpendicular to the rows. For homogeneous lattices we take all T_i's in the same form. The above definition of the T-matrix is not unambiguous and gives a lot of freedom how to choose it. We impose only one limitation on the choice of the T-matrix: the T-matrix (together with the Hamiltonian) should be invariant with respect to the transformations corresponding to the symmetry which we expect to be broken for some values of the interaction parameters. The T-matrix can obviously be written in an 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 $\sum_i G_i = H$.

It is well known that 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

$$\sum_{N_{i+k}} T_i(N_i, N_{i+1}, \ldots, N_{i+k}) \psi_1(N_{i+1}, \ldots, N_{i+k}) = \lambda_1 \psi_1(N_i, \ldots, N_{i+k-1}) \quad (3)$$

Generally, it is not possible to solve this equation exactly, as the T-matrix as well as the eigenvector are infinite along the rows. That is, why eq.(3) is usually solved only for a strip of a finite width with appropriate boundary conditions. Then, the problem turns out to be effectively one-dimensional and neither phase transitions nor spontaneous symmetry breaking appear. In our approach we leave both the T-matrix and the eigenvector infinite, but we rewrite also the eigenvector into an exponential form

$$\psi_{\iota}(N_{\iota+1},\ldots,N_{\iota+k}) = \sum_{N_{\iota+k+1}\cdots N_{\iota+k+l}} \exp\Big\{ g_{\iota+1}(\{L_p\};N_{\iota+1},\ldots,N_{\iota+k}) + h_{\iota+1}(\{J_p\};N_{\iota+1},\ldots,N_{\iota+k},N_{\iota+k+1},\ldots,N_{\iota+k+l})\Big\} \tag{4}$$

Substituting (4) into (3) we get

$$\sum_{N_{\iota+k}} \sum_{N_{\iota+k+1}\cdots N_{\iota+k+l}} \exp\Big\{ G_{\iota}(\{K_p\};N_{\iota},\ldots,N_{\iota+k}) + g_{\iota+1}(\{L_p\};N_{\iota+1},\ldots,N_{\iota+k}) + h_{\iota+1}(\{J_p\};N_{\iota+1},\ldots,N_{\iota+k},N_{\iota+k+1},\ldots,N_{\iota+k+l})\Big\} =$$

$$= \lambda_{\iota} \sum_{N_{\iota+k}\cdots N_{\iota+k+l-1}} \exp\Big\{ g_{\iota}(\{L_p\};N_{\iota},\ldots,N_{\iota+k-1}) + h_{\iota}(\{J_p\};N_{\iota},\ldots,N_{\iota+k-1},N_{\iota+k},\ldots,N_{\iota+k+l-1})\Big\} \tag{5}$$

We assume that both g_{ι} and h_{ι} can be expressed in the same way as (2) where the number of lattice sites in the cluster is finite, i.e. the number of the constants L_{ι} and J_{ι} is also finite and they are of short range. This assumption represents

the only approximation in our method; for an infinite number of the constants L_i or J_j, the expression (4) is exact. As the exponentials on the left-hand side of (4) are positive, the factorization (4) is valid only for the eigenvector corresponding to the largest eigenvalue.

If we put $h_i = 0$ we obtain a generalized mean-field approximation. Instead of a single site mean field of usual approaches, a set of many-body fields or many-body interactions $\{L_p\}$ is involved in g_{i+1} which is added to the row Hamiltonian G_i. The expression $g_{i+1}(\{L_p\};N_{i+1},\ldots,N_{i+k})$ represents the effect of the half - lattice $(N_{i+k+1},N_{i+k+2},\ldots\ldots)$ on the half - lattice $(\ldots\ldots,N_{i+k-1},N_{i+k})$. If the expression for g_i contained an infinite number of the constants L_p, all the properties of the latter half-lattice described by the Hamiltonian $H_{1\nearrow 2} = g_{i+1} + \sum_{-\infty}^{i} G_j$ would be the same as the properties of this half-lattice of the full system described by the Hamiltonian $H = \sum_{-\infty}^{\infty} G_j$. In our approximation, we assume that, in most cases, only the short-range interactions from the set $\{L_p\}$ are important (cf.approximation (i) and (ii) in Sec.3).

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

decay of those on its right-hand side. (cf. approximation (iii) in Sec.III)

The effect of the extra rows added to the left-hand side of the eigenvector is similar to the effect of the rows added to the right-hand side of both the T-matrix and the eigenvector. In this case, (5) remains unchanged, h 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. (cf.approximation (iv) in Sec.III)

Reducing only the number of interaction constants, the vector equation (5) would represent an infinite number of nonlinear equations for a finite number of unknown parameters. Thus the reduction of the number of the interaction constants L must be accompanied by the reduction of the number of the lattice sites in the strip by summing up over most of the site variables leaving only a number of equations equal to 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 consisting of $k+l$ and $k+l-1$ rows, and some of the well-known methods of the statistical mechanics can be used. 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

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

for all configurations of the lattice variables n_i of the cluster which is a part of the $(k-1)$-row strip consisting of the rows $i,\ldots,i+k-1$. P_{k+l} are the configuration probabilities of this cluster in the $(k+l)$-row statistical system described by the Hamiltonian

$$H_{k+l} = (G_i(\{K_p\};N_i,\ldots,N_{i+k}) + g_{i+1}(\{L_p\};N_{i+1},\ldots,N_{i+k}) + h_{i+1}(\{J_p\};N_{i+1},\ldots,N_{i+k},N_{i+k+1},\ldots,N_{i+k+l})$$

while P_{k+l-1} are the probabilities of the same cluster in the $(k+l-1)$-row system described by the following Hamiltonian

$$H_{k+l-1} = g_i(\{L_p\};N_i,\ldots,N_{i+k-1}) + h_i(\{J_p\};N_i,\ldots,N_{i+k-1},N_{i+k},\ldots,N_{i+k+l-1}).$$

Both probabilities are normalized to unity. The eigenvalue λ_1 has disappeared from (6) due to the normalization of the configuration probabilities. It is obtained if we sum up over all variables at both sides of (5)

$$\lambda_1 = Z_{k+l}(G_i,g_i,h_i) \,/\, Z_{k+l-1}(g_i,h_i) \qquad (7)$$

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

Eqs.(6) are the main result of this paper.

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+l} and P_{k+l-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 following Hamiltonians

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

or (8)

$$g(N_i,..,N_{i+k-1}) + g(N_{i+k-1},..,N_i) + h(N_i,..,N_{i+k-1},N_{i+k},..N_{i+k+i-1})$$
$$+ h(N_{i+k-1},..,N_i,N_{i-1},..,N_{i-l}),$$

i.e.,the multisite mean fields are now applied to both sides of the strip.

To solve (7), we use the iteration method which reminds of the power method for the matrix eigenvalue problem. Using the the values of interaction constants L_i and J_i from the preceding iteration step, the right-hand side of the equation is calculated by the T- matrix method and then the interaction constants of the next iteration step from are obtained 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_i is equal to zero (l=0) and g_i has the following explicit form:

$$g_{i+1} = \sum_j g_{i+1,j}\begin{pmatrix} n_{i+1,j},\ldots,n_{i+1,j+s_i} \\ \vdots \qquad\qquad \vdots \\ n_{i+k,j},\ldots,n_{i+k,j+s_{i+k}} \end{pmatrix}$$

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

the free energy of the $(k-1)$-row strip is the following:

$$F = \sum_j \left[\sum_{\langle n \rangle} L \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} P \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \right.$$

$$+ \sum_{\langle n \rangle} P \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \ln \left(P \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \right) \quad (9)$$

$$\left. - \sum_{\langle n \rangle} P \begin{pmatrix} n_{i+1,j+1}, \ldots, n_{i+1,j+s_i} \\ n_{i+k,j+1}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \ln \left(P \begin{pmatrix} n_{i+1,j+1}, \ldots, n_{i+1,j+s_i} \\ n_{i+k,j+1}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \right) \right].$$

The meaning of the notation in the expression for $g_{i,j}$ is analogous to that in (2). P's are the probabilities of cluster configurations in a $(k-1)$-row strip and the probabilities in the last row of (9) are obtained from them by summation over the first column; s_i is the range of the interactions L_i along the i-th row. Minimizing the free energy with respect to P's, we get the formula for the calculation of interaction constants from configuration probabilities

$$L \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} = - \ln \left(P \begin{pmatrix} n_{i+1,j}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \right) \quad (10)$$

$$+ \ln \left(P \begin{pmatrix} n_{i+1,j+1}, \ldots, n_{i+1,j+s_i} \\ \vdots \\ n_{i+k,j+1}, \ldots, n_{i+k,j+s_{i+k}} \end{pmatrix} \right).$$

There is no such a simple formula for the calculation of the constants J_i and L_i when h_i is nonzero, because of long range interactions introduced by summation over the rows

$i+k+1,\ldots,i+k+l$. To avoid this difficulty, we try to solve a larger set of equations instead of (5)

$$\sum_{N_{i+k}} \exp\Big[G_i(\{K_k\};N_i,\ldots,N_{i+k}) + g_{i+1}(\{L_p\};N_{i+1},\ldots,N_{i+k}) + h_{i+1}(\{J_r\};N_{i+1},\ldots,N_{i+k},N_{i+k+1},\ldots,N_{i+k+l})\Big] = \lambda_1 \exp\Big[g_i(\{L_p\};N_i,\ldots,N_{i+k-1}) + h_i(\{J_r\};N_i,\ldots,N_{i+k-1},\ldots,N_{i+k+l-1})\Big]. \tag{11}$$

Now, if we reduce the whole strip by summation to a cluster of the same width as that of the strip i.e.$(k+l-1)$, we can repeat the whole above described procedure for calculation of the interaction constants.

For computational reasons, it is convenient, when solving eqs.(6), to use compact clusters consisting of $k-1$ finite rows. But in principle, the cluster in (6) may be chosen arbitrarily even with sites far apart from each other. In such a way we can change the type of the approximation.

An important field of application of the described method is the 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. In these cases the symmetry breaking in the problem with a homogeneous Hamiltonian again naturally appears making all the parameters L_i, J_i site dependent. They would be periodic functions of the position with a period equal to the period of the superstructure. Now, it is more consistent to

interpret eq.(6) as a nonlinear mapping of the the parameters L_i and J_i

$$\{L_i^l\},\ \{J_i^l\} \rightarrow \{L_i^{l+1}\},\ \{J_i^{l+1}\}$$

defined by the equation (6')

$$P_{k+l}(\{L_i^l\},\{J_i^l\};n_1,\ldots,n_m) = P_{k+l-1}(\{L_i^{l+1}\},\{J_i^{l+1}\};n_1,\ldots,n_m).$$

where $\{L_i^{l+1}\}$, $\{J_i^{l+1}\}$ are shifted by one row with respect to $\{L_i^l\}$, $\{J_i^l\}$. For superstructures the repetition of the values of the parameters L_i^l, J_i^l after the number of steps equal to the period of the superstructure is expected. If the values of the parameters never repeat the system is in an incommensurate phase. The method reproduces very well the superstructures and incommensurate phases of ANNI model[14]

Our approach is, to some extent, similar to the variational approximation for square lattice models developed by Baxter[8], which can be however easily generalized to more complicated models. Despite the similarity, there are many differences between them. Baxter's method starts from the equation

$$\lambda = \frac{\Psi^T T \Psi}{\Psi^T \Psi}$$

rather than from (3); Ψ^T is for transpose of Ψ. This equation is further treated variationally.

The common feature of our and Baxter's method[8] is the factorization of the eigenvector Ψ. The factorization in Ref.8 is a special case of eq.(4). There, in our notation, $g_i = 0$ and h_i involves only interaction between two neighboring columns in the i-th row and in the l extra rows of our "mean" lattice.

The resulting equations differ from ours. In Ref.8 they

involve the transpose of Ψ_t. Generalizing the variational method to more complicated models with superstructures, it would be necessary to anticipate the periodicity of the superstructure and then to solve simultaneously a large set of matrix equations as each of the equations would combine Ψ and Ψ' for different rows. In our approach the equations are solved for each row separately. The period of the superstructure is equal to the period of the iterative nonlinear mapping procedure for the parameters L_t, J_t. It is not possible to obtain any incommensurate structures using the method in Ref.8.

Our method seems to be more natural, as the parameters L_p in g_t have a direct physical meaning of many body fields simulating the effect of one of the half-lattices on the other one, while the interpretation of J's in h_t is not so transparent.

In the iterative procedure of the variational approach all the eigenvectors and the eigenvalues of two 2^{l+1} by 2^{l+1} matrices must be calculated. In our approach, if we use the T-matrix method for calculation of P's in (6) or (6'), only the largest eigenvalue and the corresponding eigenvector are needed.

In the variational approximation, there appears a problem of "reasonable" guess of the vector ψ. In our method the choice of ψ at the beginning of the iteration procedure is not very important in those areas of the parameter space where there is no coexistence of two or more phases. It represents actually the boundary conditions for a seminfinite lattice.

As we shall see in the next Section, our approach gives better values of the critical temperature for the Ising model in low-order approximations than the variational method.

III. RESULTS FOR THE ISING MODEL

To compare the results of our approximate method with exact solutions, we calculate the critical temperature and the coverage of the two-dimensional lattice gas model on the square lattice with nearest-neighbor interactions (which is equivalent to the two-dimensional Ising model) described by the site Hamiltonian

$$H_{i,j} = K\, n_{i,j}\,(n_{i,j+1} + n_{i+1,j}) + \mu\, n_{i,j} \qquad (12)$$

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

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

We have calculated the free energy, the correlation functions, and the critical temperature for different approximations according to the following choices of the functions $G = \sum_{i,j} G_{i,j}$, $g = \sum_{i,j} g_{i,j}$, and $h = \sum_{i,j} h_{i,j}$:

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

$$g_{i,j} = \frac{L}{3}\,(n_{i,j} + n_{i,j+1} + n_{i,j+2}) + \frac{L}{2}\,n_{i,j+1}\,(n_{i,j} + n_{i,j+2}) + L_3\, n_{i,j}\, n_{i,j+2} + L_4\, n_{i,j}\, n_{i,j+1}\, n_{i,j+2}$$

$$h_{i,j} = 0$$

It is a three-site approximation.

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

$$g_{i,j} = \frac{L_1}{4}(n_{i,j}+n_{i,j+1}+n_{i,j+2}+n_{i,j+3}) + \frac{L_2}{3} n_{i,j+1}(n_{i,j}+n_{i,j+2}) +$$

$$+ n_{i,j+2} n_{i,j+3}) + \frac{L_3}{2}(n_{i,j} n_{i,j+2} + n_{i,j+1} n_{i,j+3}) +$$

$$+ L_4 n_{i,j} n_{i,j+3} + \frac{L_5}{2} n_{i,j+1} n_{i,j+2}(n_{i,j}+n_{i,j+3}) +$$

$$+ \frac{L_6}{2} n_{i,j} n_{i,j+3}(n_{i,j+1}+n_{i,j+2}) + L_7 n_{i,j} n_{i,j+1} n_{i,j+2} n_{i,j+3}$$

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

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

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

$$g_{i,j} + h_{i,j} = \frac{L_1}{2}(n_{i,j}+n_{i,j+1}) + \frac{L_2}{2}(n_{i+1,j}+n_{i+1,j+1}) +$$

$$+ \frac{L_3}{2}(n_{i,j} n_{i+1,j} + n_{i,j+1} n_{i+1,j+1}) + L_4 n_{i,j} n_{i,j+1} +$$

$$+ L_5 n_{i+1,j} n_{i+1,j+1} + L_6(n_{i,j} n_{i+1,j+1} + n_{i+1,j} n_{i,j+1}) +$$

$$+ L_7 n_{i,j} n_{i,j+1}(n_{i+1,j}+n_{i+1,j+1}) +$$

$$+ L_8 n_{i+1,j} n_{i+1,j+1}(n_{i,j}+n_{i,j+1}) + L_9 n_{i,j} n_{i,j+1} n_{i+1,j} n_{i+1,j+1}$$

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

$$\times(n_{i+1,j}+n_{i+1,j+1}) + \frac{K}{3}(n_{i,j} n_{i,j+1} + n_{i+1,j} n_{i+1,j+1} + n_{i+2,j} n_{i+2,j+1})$$

$$+ \frac{K}{4}(n_{i+1,j}(n_{i,j}+n_{i+2,j}) + n_{i+1,j+1}(n_{i,j+1}+n_{i+2,j+2})$$

$h_{i,j} = 0$

$g_{(\ldots)}$ is equal to $g_{(\ldots)} + h_{(\ldots)}$ in (iii).

The specific 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 $T_{(\ldots)}=\exp(G_{(\ldots)})$ with respect to the particle-hole symmetry when $\mu=-2K$ (i.e. the magnetic field is equal to zero for the corresponding Ising spin model). The clusters, on which the functions $G_{(\ldots)}$, $g_{(\ldots)}$, and $h_{(\ldots)}$ are defined, are shown in Fig.1.

The values of the critical temperature (the critical pair interaction $K_c = J/k_B T_c$) for the approximations (i-iv) together with the exact value are given in Tab.1. They are the largest values of the pair interaction when the coverage $\langle n \rangle$ is still equal to $\frac{1}{2}$. The coverage is calculated from the correlation functions of a one-dimensional system described by the Hamiltonian (8). 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 $\frac{1}{2}$ (the magnetization is nonzero). As our method is of mean-field type with the critical exponent of magnetization $\beta=\frac{1}{2}$ instead of the real value $\frac{1}{8}$, 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.2. 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.

Baxter's variational method has been applied to the Ising model by Tsang[9]. For the special case of magnetic field equal to zero, he has been able to find the critical temperature for the first 20 approximations using Kaufman's technique of spin representation. We have performed the calculations only for few first approximations using a quite general approach applicable to any Hamiltonian with short-range interactions. Our approximation (iv) with 4-site clusters in $g_{i,j}$, which corresponds to Tsang's n=4 approximation, yields better results for the critical temperature ($K_{c,IV}$ = 1.7638) than the variational method ($K_{c,4}$ = 1.7580) ($K_{c,exact}$ = 1.7627).

In conclusion, we have developed an approximate method for the calculation of thermodynamic 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 it has been shown for the Ising model, the results of the method are very close to the exact results, even in the case of 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. As the method is reformulating the calculation of the partition function to a

nonlinear mapping of the effective multisite fields acting on the strip of the rows $i,\ldots,i+k$ to the fields acting on the strip of the rows $i-1,\ldots,i+k-1$, the superstructures and incommensurate phases appear from the calculations quite naturally[14]

ACKNOWLEDGEMENTS

The author would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. He would also like to thank Professor E.Tosatti for critical reading of the manuscript, discussion and valuable remarks.

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TABLE I. Critical interaction constant for the Ising model in our approximations and its exact value.[13]

$K_{c,I}$	$K_{c,II}$	$K_{c,III}$	$K_{c,IV}$	$K_{c,exact}$
1.775	1.7672	1.7652	1.7638	1.7627

Figure captions.

Fig. 1. Clusters of sites on which the functions $G_{i,j}$ (squares with vertical bars) and $g_{i,j}$, $h_{i,j}$ (squares with horizontal bars) for the approximations (i) - (iv) are defined.

Fig. 2. Coverages for the lattice-gas Ising model in our approximations and their exact values.[13] The coverages in the approximation (iii) lie between the values of the approximations (ii) and (iv).

Fig.1

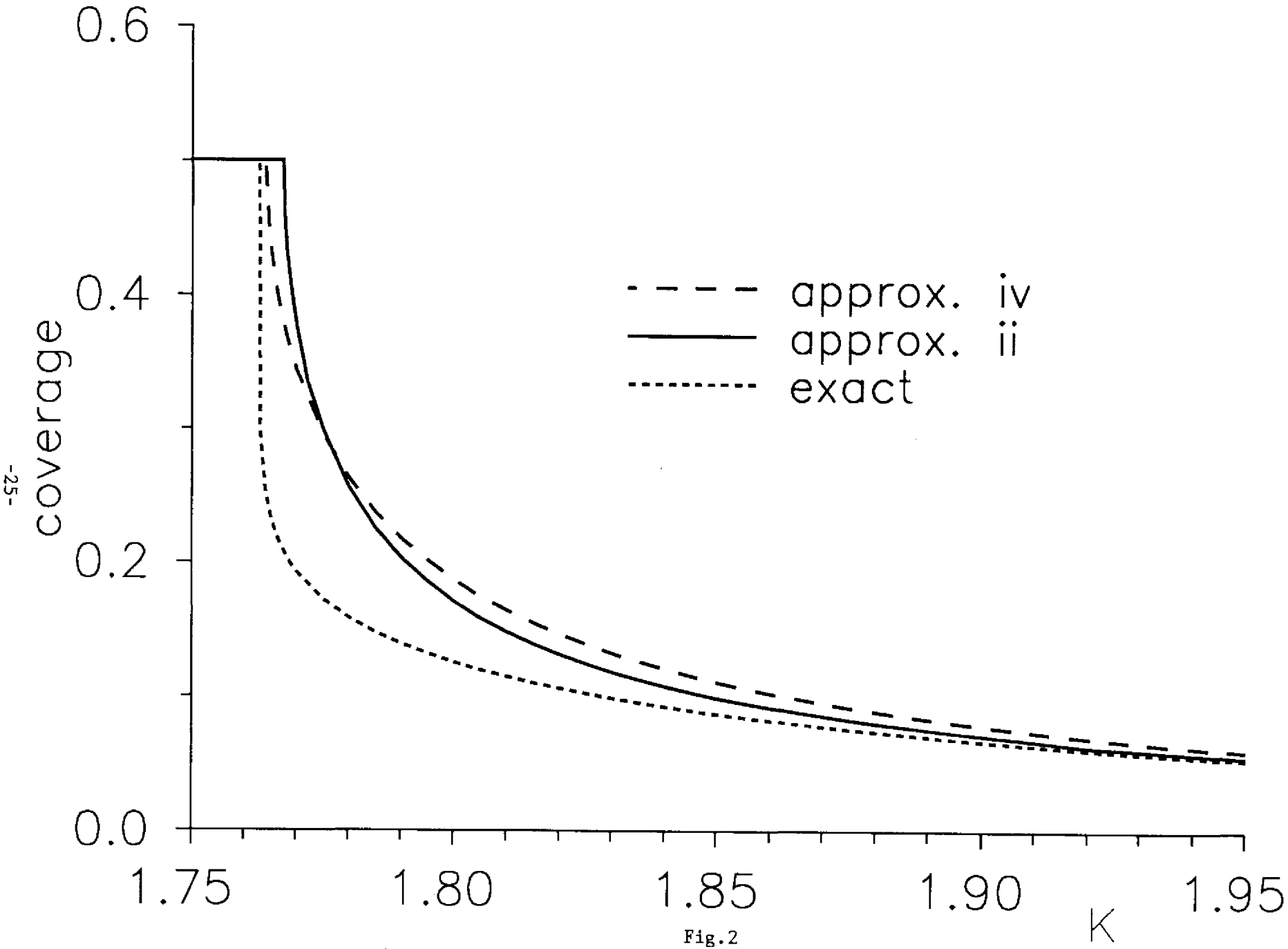
0.6
0.4
0.2
0.0
coverage
1.75
1.80
1.85
1.90
1.95
K
approx. iv
approx. ii
exact

Fig.2

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