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A renormalisation-group method for lattice gas models

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Abstract. A new method for calculating the critical temperature and critical exponents of classical discrete models, based on the renormalisation-group method and the cluster variational method, is developed. In the lowest approximation, using the mean field approximation and quasichemical approximation, the results for the two-dimensional Ising model are obtained within 2% accuracy.

The recent progress in experimental investigation of order–disorder phase transitions in physisorbed and chemisorbed systems has stimulated a great deal of interest in calculations of critical properties of two-dimensional lattice gas models which are assumed to be a good approximation of real adsorbates on crystal surfaces. A good basis for such calculations is the real-space renormalisation-group method devised by Niemeijer and van Leeuwen (1974) that has made great progress since then (Burkhardt and van Leeuwen 1982). All the real-space renormalisation-group methods (except for phenomenological approaches) developed till now make use of the Gibbs formulation of statistical mechanics, and the central thermodynamic quantities of interest are the partition function and the free energy. The various methods differ in the choice of the weight function determining the renormalisation-group (RG) transformation and in the choice of the approximative treatment of the partition function. Our approach is based on the correlation functions or the probabilities of state of a finite cluster of an infinite lattice which are approximatively calculated by the cluster variation method (CVM). In the choice of the weight function of the RG transformation we follow the majority rule of Niemeijer and van Leeuwen (1974) and Nauenberg and Nienhuis (1974).

Our method yields surprisingly good results even in the lowest approximation, far exceeding in accuracy the results obtained with the same effort by other authors.

We believe that this high accuracy originates in some features of our approach where, using CVM results with broken symmetry, we are able to make use of the information which is contained in the values of small odd correlation functions which in the other approaches possess trivial values equal to zero.

For the sake of symmetry we shall develop the method for an Ising spin system instead of the lattice gas directly, and its description will be formulated in terms of probabilities of spin configurations (which are, in fact, the correlation functions of lattice gas occupation number operators).

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Let the system be described by the Hamiltonian

$$H = K_1 \sum_{NN} s_i s_l + K_2 \sum_{NNN} s_i s_l + \ldots + k_j \sum s_i s_l \ldots s_n + h_1 \sum s_i + h_2 \sum s_i s_l s_n + \ldots + h_k \sum s_i s_l \ldots s_n = H_e + H_o \tag{1}$$

where the even part H_e contains only the sums of products of an even number of spin variables and the part H_o contains only the products of an odd number of spin variables and $s_n = \pm 1$. The average values of the products of spin variables (correlation functions) which appear in (1) will be further denoted by C_i. The correlation functions C_i are simply related, by means of linear formulae, to the probabilities P_i of all possible configurations of spins defined on the cluster of sites which contains all the clusters appearing in (1). These probabilities can be found for any given set of coupling constants K_i, h_i using some version of CVM (Kikuchi 1951, Kikuchi and Brush 1967, Šurda 1982, Šurda and Karasová 1983). The method is based on the minimisation of the free energy $F = \langle H \rangle - TS$, where both the average value of the energy $\langle H \rangle$ and the entropy S are expressed approximately by the probabilities P_i. As was shown, CVM describes well the behaviour of thermodynamic and correlation functions everywhere but the close vicinity of critical points. To improve the results in this region, we have to use some RG ideas.

We shall develop the method first for the case of a ferromagnetic phase transition, where the critical points lie in the subspace $h_i = 0$ of the coupling-constant space. In the approximation based on a cluster with r sites we divide the whole lattice into cells each consisting of l^d sites and take a cluster consisting of r cells. For a given set of coupling constants K_i, $i = 1, \ldots, s$, we calculate all the probabilities P_i defined on the cluster of cells by CVM. Then we apply to the obtained probabilities an RG transformation satisfying the majority rule (Nauenberg and Nienhuis 1974). The transformation can be written in the following way:

$$P_i' = \sum_n U_{in} P_n, \qquad i = 1, \ldots, s. \tag{2}$$

Using again the equations of CVM we calculate new coupling constants K_i' corresponding to the probabilities P_i'. In this way one RG step from the coupling constants K_i to the set of constants K_i' was performed. The equality $K^{*\prime} = K^*$ determines the fixed point of the transformation. We see that CVM was used twice in the RG procedure: first in calculating the probabilities P_i and second in obtaining the constants K_i'. It is essential for our approach that in the first application we have to use CVM involving larger clusters (i.e. the higher approximation) than in the second case. That means that not only is the lattice scaled in the process of calculation but also the order of approximation. In the paramagnetic phase all the odd correlation functions are equal to zero when $h_i = 0$. Then the number of independent probabilities is equal to the number of even coupling constants. In the ferromagnetic phase (where the non-trivial fixed point occurs) the situation is different. There the symmetry is broken and all the even and odd correlation functions are non-zero. To preserve the correspondence between the coupling constants and probabilities we have to increase the number of even coupling constants to $s = j + k$, where j and k are the numbers of even and odd coupling constants in (1), respectively. Now the range of interaction is larger than the diameter of the largest cluster. Thus, evaluating K_i' from P_i', we have to use a higher

approximation of CVM to preserve all probabilities of state of large clusters entering into $\langle H \rangle$ and determine the superfluous probabilities from the requirement of minimum free energy, or we have to determine the order of CVM only by the largest cluster obtained from the RG procedure and express the probabilities of the large clusters in $\langle H \rangle$ in terms of smaller ones using the method described in Šurda (1982). In the illustrative calculations below we shall use the second possibility.

Taking into account that the RG transformation based on the majority rule makes the absolute values of non-zero odd correlation functions larger, and the fact that the absolute values of critical coupling constants K_i^c increase with the order of approximation, we see that the non-trivial fixed point of the transformation is in the ferromagnetic region of the coupling-constant space not far from the phase transition of the better of our two approximations, and it converges together with CVM critical values to the exact critical surface for higher approximations. It is important that for the low approximations the fixed point is not too close to the CVM phase transition plane, because the method does not work well in this area. The temperature critical exponent y_T is calculated in an ordinary way from the linearised RG transformation at the fixed point.

On the other hand, having more coupling constants than probabilities of state, we cannot obtain the RG trajectories in the whole coupling-constant space. However, with the same success as in the even subspace the procedure can be applied also to the odd subspace containing the fixed point $(K^*, h^*) = (K_1^*, K_2^*, \ldots, K_j^*, 0, 0, \ldots, 0)$. In the same way we obtain the transformation for $j+k$ odd constants h_j and the magnetic critical exponent y_h.

The treatment of the antiferromagnetic phase transition is similar to that mentioned above. Now, we have only to change the sign of spins in one of two sublattices in both the old and new lattice before application of the majority rule in the RG transformation. The number of probabilities is now larger than in the previous case due to the presence of two sublattices. Thus, in order not to enlarge the number of coupling constants, only the probabilities P'_{1i} for one sublattice are obtained from the majority rule. The probabilities P'_{2i} for the other sublattice are calculated from CVM equations. However, in the absence of the magnetic field the probabilities P'_{2i} can be directly expressed in terms of probabilities P'_{1i} of the other sublattice. Hence, the number of independent probabilities is only $j+k$ and it can be shown that the problem becomes equivalent to the ferromagnetic phase transition with the same fixed point and critical exponent y_T. In the system with the magnetic field the equivalence is lost and y_h becomes negative. In a similar way the majority rule can be applied to systems with other types of superstructure.

Recently, there has appeared another simultaneous application of CVM and real-space renormalisation group (Hecht and Kikuchi 1982) to the calculation of critical properties of lattice spin systems. That approach, in spite of using the same kind of computational method, differs from our one substantially. It is closely related to the original method by Niemeijer and van Leeuwen (1974), but calculating RG transformations for a finite number of coupling constants, an infinite lattice with an infinite number of fixed cell spins, instead of a finite lattice, is used. As the results of the method depend on an arbitrary choice of configuration of superfluous cell spins, a number of critical exponents and critical temperatures instead of one set of exponents and one critical temperature is obtained. The RG transformations are derived from expressions for the free energy of the system with fixed cell spin configurations. In our approach there is no need for calculation of the free energy. In our opinion, our

method, which is based on an approximative calculation of correlation functions of systems of spins and cell spins in thermal equilibrium better describes the system near the critical region than the above mentioned one where expressions for the free energy of a spin system satisfying an infinite number of constraints are used.

In order to give a simple illustration of our approach, we shall calculate the critical properties of the two-dimensional ferromagnetic Ising model on a square lattice in the lowest approximation. In this approximation our method is similar to the lowest approximation of the MFA method of Indekeu *et al* (1982).

In our simple scheme only one odd correlation function (magnetisation), one-dimensional even and odd coupling-constant space given by the NN pair interaction K and the magnetic field h are taken into account. The cell spin s_i' is placed in the centre of a square of four spins, i.e. the scale factor $l = 2$. To calculate the magnetisation or probability of state of a site with the spin directed up, CVM based on the one-site cluster—the mean field approximation—is used. The cluster of cells is represented by one cell of four spins which probabilities of state have to be calculated by a higher-order approximation of CVM than MFA.

Let us denote the probability of state of a given configuration of spins occupying a square of lattice sites by P_4. Then, the majority rule can be expressed explicitly as follows:

$$P_1'(+) = P_4(++++) + P_4(+++-) + P_4(++-+) + P_4(+-++) + P_4(-+++) + P_4(++--) + P_4(+--+) + P_4(+-+-) \tag{3}$$

where the signs in the argument denote the signs of spins at sites of the square beginning from the right upper corner which determines the sign of the cell spin when $\Sigma s_i = 0$ (Nauenberg and Nienhuis 1974). Using the normalisation condition for probabilities, the number of terms in (3) can be reduced,

$$P_1'(+) = P_2(++) + P_3(+-+) + P_3(++-), \tag{4}$$

where P_2 and P_3 are the probabilities of state of a nearest-neighbouring pair cluster and of a three-site cluster, respectively. Using the relation in Šurda (1982), the three-site clusters can be factorised:

$$P_1'(+) = P_2(++) + P_2^2(+-)/P_1(-) + P_2(++)P_2(+-)/P_1(+). \tag{5}$$

The same arithmetic yields also an expression for the probability of a negative sign of the cell spin:

$$P'(-) = P_2(--) + P_2^2(+-)/P_1(-) + P_2(--)P_2(+-)/P_1(+).$$

After a short manipulation it is seen that our approximation conserves the normalisation condition

$$P_1'(+) + P_1'(-) = 1. \tag{6}$$

The factorisation in (5) is based on the idea that two NNN spins s_1, s_2 with a fixed spin s_3 between them are to some extent independent and the conditional probability in their state can be expressed as a product of conditional probabilities of states of spins s_1, s_2:

$$P_3(s_1 s_3 s_2)/P(s_3) = (P_2(s_1 s_3)/P(s_3))(P(s_3 s_2)/P(s_3)). \tag{7}$$

This relation is the lowest approximation to an exact equality in which an infinite line

of fixed spins should replace s_3. The approximation (7) is also used when one derives the quasichemical approximation (QCA) from the higher CVM approximation (Šurda 1982). Thus, QCA is the most suitable method for calculation of spin system probabilities which appear in (5) being of the same order of accuracy. QCA is given by the following two equations:

$$P_2(++)P_2(--) = e^{-4K}P_2^2(+-), \qquad P_2^2(++)/P_1^3(+) = e^{-2h}P_2^2(--)/P_1^3(-). \tag{8}$$

The cell spin system is described by MFA,

$$2h' - 8K' + 16K'P_1'(+) = -\ln P_1'(+)/P_1'(-). \tag{9}$$

The two approximations, MFA and QCA, are the two lowest CVM approximations and can easily be obtained from the general formulation of CVM (Šurda 1982, Šurda and Karasová 1983). On the other hand they have been well known for a long time. Their combinatorial derivation is described e.g. by Hill (1956).

To get the relation between K' and K and between h' and h we have to solve (5), (6), (8) and (9) together with the normalisation conditions

$$P_1(+) = P_2(++) + P_2(+-), \qquad P_1(+) + P_1(-) = 1,$$
$$P_2(++) + 2P_2(+-) + P_2(--) = 1. \tag{10}$$

Performing the calculation first in the even subspace, we put $h = h' = 0$ and $K = K' = K^*$. To obtain the unknown probabilities $P_{1,2}$, P_1' and the fixed point value of the coupling constant K^*, we have to solve the nonlinear system of equations (5), (6), (8), (9) and (10) numerically. (In fact, it may be reduced to only one nonlinear equation.) Having the value of K^*, we perform the derivative of all equations with respect to K at the fixed point $K = K^*$, $h = 0$. From the resulting system of linear equations the value of $(\partial K'/\partial K)_{K=K^*,h=0}$, which is equal to an exponential function of the thermal critical exponent 2^{y_T}, is obtained.

Similarly, in the odd subspace, after performing the derivation with respect to h at the fixed point, the system of linear equations yields $(\partial h'/\partial h)_{K=K^*,h=0} = 2^{y_h}$.

The results are given in the following table, where also the exact results are presented for comparison.

	Our results	Exact results
K_c	0.442	0.441
y_T	1.000	1
y_h	1.842	1.875

Comparing our results with results requiring the same effort of other authors (Niemeijer and van Leeuwen 1974, Indekeu *et al* 1982), we see that an improvement of about an order has been obtained.

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