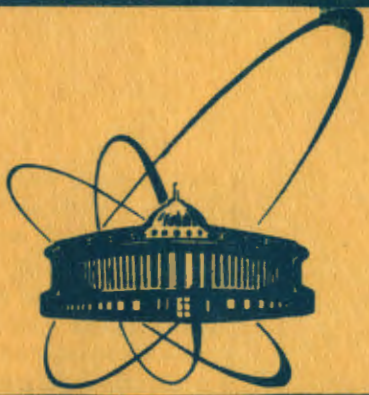

сообщения
объединенного
института
ядерных
исследований
дубна

E17-83-682

A.Šurda

CALCULATION OF CRITICAL PROPERTIES OF LATTICE GAS MODELS

1983

The recent progress in experimental investigation of order-disorder phase transitions in physisorbed and chemisorbed systems has stimulated a great deal of interest in calculation 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 renormalization group method devised by Niemeyer and van Leeuwen/1/ in 1973 that has made a great progress since then/2/. All the real-space renormalization-group methods (except of 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. Various methods differ in choice of the weight function determining the renormalization group (RG) transformation and in choice of the approximative treatment of the partition function. Our approach is based on the correlation functions or on 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 the authors/1,3/.

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.

For the sake of symmetry we shall develop the method for an Ising spin system instead of the lattice gas directly and its general description will be formulated in terms of correlation functions.

Let the system be described by the Hamiltonian

$$H = K_1 \sum_{n.n} \sigma_n \sigma_m + K_2 \sum_{n.n.n} \sigma_n \sigma_m + \dots + K_j \sum \sigma_n \sigma_m \dots \sigma_t + \\ + h_1 \sum \sigma_n + h_2 \sum \sigma_n \sigma_m \sigma_t + \dots + h_k \sum \sigma_n \sigma_m \dots \sigma_t \equiv H_e + H_0 , \tag{1}$$

where the even part H_e contains only the sum of products of even number of spin variables and the odd part H_0 contains only the products of odd number of spin variables and $\sigma_i = \pm 1$. The average values of the products of spin variables (correlation functions) which appear in (1) will be further denoted by C_i^e or C_i^o, for even and odd correlation functions, respectively ($C_1^o = \langle \sigma_i \rangle$, $C_1^e = \langle \sigma_i \sigma_j \rangle$). These correlation functions can be

found for any given set of coupling constants K_i, h_i using some version of CVM /4-7/. The method is based on the minimalization 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 correlators C_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 renormalization group ideas.

The main principles of our approach follow the general ideas of real-space renormalization-group method. We shall develop them at first for the case of 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^2 sites and take a cluster consisting of r cells. For a given set of coupling constants K_i, $i = 1,...,s$ we calculate all the correlation functions S_i defined on the cluster of cells by CVM. Then we apply to the obtained correlation functions an RG-transformation satisfying the majority rule /1,3/. The transformation can be written in the following way

$$C_i' = \sum_n P_{in} S_n \qquad i = 1,...,s. \tag{2}$$

Using again the equation of CVM we calculate new coupling constants K_i' corresponding to the correlation function C_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 correlation functions S_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 the lattice is scaled in the process of calculation but also the order of approximation.

In the paramegnatic phase all the odd correlation functions are equal to zero. Then the correlation functions, which appear in (2), are even and the number of even coupling constants is equal to the number of even correlation functions, i.e., $j = s$. In the ferromagnetic phase (where the nontrivial fixed point occurs) the situation is different. There the symmetry is broken and all the even and odd correlation functions are nonzero. To preserve the correspondence between the coupling constants and correlation functions we have to increase the number of the even coupling constants to $s = j + k$. Now the range of interaction is larger than the diameter of the largest cluster. Thus,

evaluating K_i' from C_i', we have to use a higher approximation of CVM to preserve all correlation functions of large clusters entering into $\langle H \rangle$ and determine the superfluous correlation functions from the requirement of minimum of the free energy or we have to determine the order of CVM only by largest cluster obtained from the RG procedure and express the correlation functions of the large clusters in $\langle H \rangle$ in terms of smaller ones using the method described in /6/. In the illustrative calculation below we shall use the second possibility.

Taking into account that the RG transformation based on the majority rule makes the absolute values of nonzero 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 nontrivial fixed point of the transformation is in the ferromagnetic region of the coupling-constant space not far from the phase-transition plane of the better one 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 two close to the CVM phase transition plane, because the method does not work in this area well. The temperature critical exponent is calculated in the ordinary way from the linearized transformation at the fixed point.

On the other hand, having more coupling constants than correlation functions 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 $(K^*, h^*) \equiv (K_1^*,...,K_j^*,0,...,0)$. In the same way we obtain the transformation for $j + k$ odd constants h_i 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 correlation functions is now larger than in the previous case due to the presence of two sublattices. Thus, besides $j + k$ even coupling constant we have to add some odd constants to the coupling-constant space in order to match the number of them and the number of correlation functions. However, in the absence of the magnetic field the correlation functions in different sublattices differ only by the sign. The number of independent correlation functions is only $j + k$ and it can be shown that the problem becomes equivalent in 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 the systems with other types of superstructure.

In fact, CVM and the majority rule are formulated more straightforwardly in terms of probabilities of state of a cluster with a given configuration of spins than in terms of correlation functions. For that reason we use in the following simple calculation the formalism of probabilities of state. On the other hand, for higher approximations it can obscure the situation, because the odd- and even-correlation function subspaces are mixed.

To give a simple illustration of our approach, we shall calculate the critical properties of the 2-dimensional ferromagnetic Ising model in a square lattice in the lowest approximation. In this approximation our method is similar to the lowest approximation of the MFA method /8/.

In our simple scheme only one odd correlation function (magnetization), 1-dimensional even and odd coupling constant space given by the n.n. pair interaction K and the magnetic field h are taken into account. The cell spin σ_i' is placed in the centre of a square of 4 spins, i.e., the scale factor $\ell = 2$. To calculate the magnetization or a 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 in our case is one cell of 4 spins, which probabilities of state have to be calculated by a higher order approximation of CVM than MFA. For the sake of simplicity we do not use CVM based on a 4-site cluster, but only on a 2-site cluster - the quasi-chemical approximation.

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. Using the normalization 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 3-site cluster, respectively. Using the relation in /6/ the 3-site clusters can be factorized

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

To get the relation between K' and K and between h' and h we have to solve, together with (5), the following MFA and QCA equations

$$2h' - 8K' + 16K' P_1'(+) = -\ln \frac{P_1'(+)}{P_1'(-)},$$

$$P_2(++)\,P_2(--) = e^{-4K} P_2^2(+-), \tag{6}$$

$$\frac{P_2^2(++)}{P_1^3(+)} = e^{-2h} \frac{P_2^2(--)}{P_1^3(-)}.$$

In the even subspace the fixed point K* from (6) and the critical exponent y_T from $2^{y_T} = \frac{\partial K'}{\partial K}$ can be found. Fixing $K = K^*$, the magnetic critical exponent can be derived from $2^{y_h} = \frac{\partial h'}{\partial h}$ in the odd subspace. The simple numerical calculation has been performed by using a pocket calculator. The results are given in the following table, where also the exact results are presented for comparison.

Table

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

Comparing our result with the results requiring the same effort of the other authors /1,8/, we see that an improvement of about an order has been obtained.

REFERENCES

1. Niemeijer Th., van Leeuwen J.M.J. Physica, 1974, 71, p.17.
2. Real-Space Renormalization. (Eds. T.W.Burkhardt, J.M.J. van Leeuwen). Springer-Verlag, 1982.
3. Nauenberg M., Nienhuis B. Phys.Rev.Lett., 1974, 33, p.344, 1598.
4. Kikuchi R. Phys.Rev., 1951, 81, p.988.

5. Kikuchi R., Brush S.G. J.Chem.Phys., 1967, 47, p.195.
6. Šurda A. Z.Phys.B, 1982, 46, p.371.
7. Šurda A., Karasová J. Czech.J.Phys. (to be published).
8. Indekeu I.O., Maritan A., Stella A.L. J.Phys.A, 1982, 15, p.L291.

Received by Publishing Department
on September 28,1983.

SUBJECT CATEGORIES OF THE JINR PUBLICATIONS

Index	Subject
1.	High energy experimental physics
2.	High energy theoretical physics
3.	Low energy experimental physics
4.	Low energy theoretical physics
5.	Mathematics
6.	Nuclear spectroscopy and radiochemistry
7.	Heavy ion physics
8.	Cryogenics
9.	Accelerators
10.	Automatization of data processing
11.	Computing mathematics and technique
12.	Chemistry
13.	Experimental techniques and methods
14.	Solid state physics. Liquids
15.	Experimental physics of nuclear reactions at low energies
16.	Health physics. Shieldings
17.	Theory of condenced matter
18.	Applied researches
19.	Biophysics

Шурда А. E17-83-682
Вычисление критических свойств модели решеточного газа

Получен новый метод для вычисления критической температуры и критических экспонент для классических дискретных моделей. Предложенный подход использует идеи метода ренормгруппы и кластерный вариационный метод. В низшем приближении с помощью аппроксимации среднего поля и квазихимической аппроксимации для двумерной модели Изинга получены результаты с точностью до 2%.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1983

Šurda A. E17-83-682
Calculation of Critical Properties of Lattice Gas Models

A new method for calculation of critical temperature and critical exponents of classical discrete models is developed. The ideas of the renormalization group method and the cluster variational method are used. In the lowest approximation, the results within 2% accuracy are obtained for 2-dimensional Ising model.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1983