ON A FACTORIZATION OF THE KINETIC ISING MODEL

B. MAMOJKA1), Bratislava

Using the principle of the maximal information entropy, a set of factorization of probabilities of states for kinetic Ising models is deduced. The properties of factorization are studied. We find the connection between the approximation based on our factorization and the Hamiltonian of the corresponding equilibrium Ising model.

О ФАКТОРИЗАЦИИ КИНЕТИЧЕСКОЙ МОДЕЛИ ИЗИНГА

В работе при использовании принципа максимальной энтропни информации выведена совокупность факторизации вероятностей состояний для кинетических моделей Изинга. При этом изучаются свойства данной факторизации. Найдена связь между приближением, основанном на данной факторизации, и гамильтонианом соответствующей равновесной модели Изинга.

I. INTRODUCTION

In order to solve the kinetic Ising model it is often necessary to factorize the probability distributions of the states of the whole system by means of the probability distributions of the states of its suitably chosen subsystems. There is e.g. [1]). In this article we study the factorization P(M(S)) of the probability distribution of the states M(S) of a spin system $(s_i = 1 \text{ or } -1)$ on a lattice M. The states x(S) on the clusters x from the suitably chosen set x of clusters on the lattice axioms based on the principle of the maximal entropy. It is also the consequence of the corresponding equilibrium Hamiltonian.

Performing the calculations with out factorization we found two important sults:

¹) Institute of Physics, Electro-Physical Research Centre, Slov. Acad. Sci., Dúbravská cesta, 842 28 BRATISLAVA, Czechoslovakia.

- to obtain the correct equilibrium solution using the approximation based on our 1. The necessary condition imposed on the structure of the set X which enables
- equilibrium state of a certain time-dependent Hamiltonian at a fixied time t which goes to the corresponding equilibrium Hamiltonian for t. our factorization is such as if at any time t the system were in an instantaneous 2. The time development of the studied kinetic Ising model obtained by use of

phase transition [13, 14, 15]. the methods using computer simulations of the growth of a new phase during the 11, 12] by means of the method of the renormalization group as well as by means of simultaneously with experimental observations of a surface diffusion, adsorption, the behaviour of kinetic models has been mainly studied in the critical region [10, been commonly used which are typical for the thermal equilibrium [8, 9]. Recently, desorption and chemical reactions. In order to describe these effects methods have [7]. The theoretical investigation of the kinetic lattice models has been carried out as the other ones, based on Green's function method, are described in the survey procedures have been proposed for their study [4, 5, 6]. These procedures, as well except for the simplest possible one, were not solved exactly, several approximative subject has been intensively studied. As even such simple version of kinetic models, rium states of which are equivalent to those of the corrresponding Ising models, the since Glauber [17] formulated his wellknown simple kinetic models, the equilibdescribe adsorption and desorption of gases on the surface of crystals [2], [3]. Only Originally, some simple kinetic lattice models have been studied in order to remain very important objects for the theoretical investigation of the Ising systems. a deeper understanding and justification of some used factorizations. These models We have centred our attention on the kinetic Ising models in order to gain

II. FACTORIZATION

To obtain our factorization we postulate the following axioms: A₁. The probabilities P(x(S)), $x \in X$ are known.

A2. There are known all the momenta

$$m_z = \sum_{M(S)} \prod_{i \in z} s_i P(M(S)), \qquad z \in X'$$
 (1.a)

$$X' = \{z | z \subseteq x, \ x \in X\} \tag{1.b}$$

generated by the probabilities P(x(S)), $x \in X$. The index i numbers the lattice points. The axiom A_2 is equivalent to A_1 .

B. We have no information on the probabilities P(y(S)), $y \notin X'$.

C. The missing information on the probabilities P(y(S)), $y \notin X'$, is replaced by

the demand for the maximum entropy of the factorized probability distribution

models, the time development of which is described by the kinetic equations These axioms can be applied to the approximative solution of the kinetic Ising

$$\frac{\mathrm{d}}{\mathrm{d}t}(P(y(S))) = F_y(M(S)), \quad y \subseteq M \tag{2.a}$$

equations. To solve Eq. (2.a) approximately we must take only some subsystem of the system, for which we write $P(z(S)), z \subseteq M$. In the majority of cases we can not solve exactly this system of Where $F_r(M(S))$ are functionals depending generally on all the probabilities

$$\frac{\mathrm{d}}{\mathrm{d}t}(P(x(S))) = F_x(M(S)), \quad x \in X,$$
(2.b)

set of all pairs of nearest neighbours) create the basis of the approximation applied factorization (e. g. using the axioms A.—C.) and the choice of the set X (e. g. the approximative solution of the system of the kinetic equations (2.a). The choice of to the solution to the given problem. through the axiom A1. Thus we have obtained the selfconsistent method for an P(x(S)), $x \in X$. These are then used as an input in our factorization procedure (2.b) we obtain the system of equations for the calculation of the probabilities means of the probabilities P(x(S)), $x \in X$. Inserting these factorizations into Eq. system (2.b) closed we have to express all the probabilities P(y(S)), $y \notin X'$ only by which do not appear on the left-hand sides of the Eqs. (2.b). In order to make the functionals $F_x(M(S))$, $x \in X$ still depend on all the probabilities P(y(S)), $y \notin X'$ where X is the suitable set of clusters on M mentioned in the axiom A_1 . The

A2., B., and C. We look for the maximum of the entropy In order to find the actual form of the wanted factorization, we use first axioms

$$W = \sum_{M(S)} P(M(S)) \ln P(M(S))$$

ω

satisfying the condition (1.a). Then the variational method gives

$$P(M(S)) = \exp\left[\sum_{z \in X_{-}} q_{z} \prod_{i \in z} s_{i}\right] / Z, \tag{4.a}$$

where Lagrange's multiplicators are given as follows

$$m_{t} = \frac{\partial \ln Z}{\partial q_{t}} \tag{4b}$$

$$Z = \sum_{M(S)} \exp\left[\sum_{i \in X} q_i \prod_{i \in I} s_i\right]. \tag{4.c}$$

From the formula (4.a) it also follows directly that

$$\sum_{\mathbf{M}(S)} \prod_{i \in z} s_i \ln P(\mathbf{M}(S)) = \begin{cases} q_z & \text{if } z \in X' \\ 0 & \text{otherwise.} \end{cases}$$
 (5)

We can obtain the same equations by means of extremalization of entropy (3) with respect to the unknown momenta m_c , $z \notin X'$. In this procedure the following expression of the probability distributions is used

$$P(M(S)) = \sum_{M(T)} \prod_{i \in M} \left[\frac{1}{2} (1 + s_i t_i) P(M(T)) \right] = \left(\frac{1}{2} \right)^N \left(1 + \sum_i m_i s_i + \sum_{i \neq j} m_{ij} s_i s_j + \dots \right),$$

where N is the number of lattice points.

The exponent in the formula (4.a) is a Hamiltonian of the Ising model with the interactions — kTq_t of the spins within the range of the cluster $z \in X'$. This fact points to the correspondence between the applied approximation — namely the choice of the set X — and the Hamiltonian of the studied system in its thermal equilibrium. Let this Hamiltonian be of the form

$$H = -\sum_{u \in U} K_u \prod_{i \in u} s_i. \tag{7}$$

The applied factorization (4.a) enables us to obtain an approximative solution achieving an equilibrium state only if the following condition is satisfied

Only in this case is it possible to require the satisfaction of the following conditions

$$\lim_{t \to +\infty} q_u(t) = -K_u/kT \text{ for all } u \in U$$
 (9)

 $\lim_{t \to +\infty} q_i(t) = 0 \text{ otherwise.}$

The condition (8) sets up the important requirements on the choice of the set X because the set X' is unambigously determined by the set X by means of the formula (1.b). The choice of a set X larger than required by conditions (8) can improve the approximation but simultaneously the calculations are more cumbersome.

It is sometimes more convenient to use another expression for the factorization (4) based on the axioms A₁, B and C. In this case we use the conditions

$$P(x(S)) = \sum_{x(S)} P(M(S)), \quad x \in X$$
 (10)

instead of the condition (1.b), x is the complement to the x in M. In this case the variational method gives

$$P(M(S)) = \exp\left[\sum_{x \in X} L_x(S)\right]$$
(11)

20

$$P(M(S)) = \prod_{x \in X} l_x(S), \quad l_x(S) = \exp[L_x(S)], \tag{12}$$

where Langrange's multiplicators $L_*(S)$ depend only on spins in the cluster x. Since, e.g.

$$L_x(S) + L_y(S) = L_x'(S) + L_y'(S)$$

 $L_x'(S) = L_x(S) + v_{x \cap y}(S)$

$$L'_{\nu}(S) = L_{\nu}(S) - v_{x \cap \nu}(S),$$

the functions $L_x(S)$ are not unambiguous. Here $v_{x \cap y}(S)$ is an arbitrary function of spins on the interaction of sets x and y. The expressions (4), (11), (12) are equivalent to each other. That can be easily shown by expanding $L_x(S)$ into the spin series.

The most eirect way to find the explicit form of the factorization (4.a) is to calculate q_z , $z \in X'$ as functions of P(x(S)), $x \in X$ or m_z , $z \in X'$. As we shall see later on this procedure is too cumbersome.

We are able to solve it successfully only in one dimension and for special quasi-one dimensional models. In spite of this fact it is possible to derive some generally valid properties of the factorization for any dimension.

Let us define the neighbourhood B_u of the cluster u as follows

$$B_u = C_u - u \tag{13.a}$$

$$C_{\nu} = \bigcup_{z \in X_{\nu}} z \tag{13.b}$$

$$x_{u} = \{z \mid z \cap u \neq \emptyset, \ z \in X\}. \tag{13.c}$$

Thus the neighbourhood B_u is the set of all the lattice points which do not belong to u but belong at least to one cluster $z \in X$ such that $z \cap u \neq \emptyset$. This neighbourhood is unambigously determined by the set X. If the set X is chosen as the smallest, satisfying the requirement (8), then the neighbourhood B_u represents the range of interaction of spins belonging to the cluster u.

Let us study the properties of the conditional probability $P(u(S)|(\overline{u \cup v})(S))$ where $u \cap v = \emptyset$. Using the definition (13) and the factorization (12) we obtain

$$P(u(S)|\overline{(u \cup v)}(S)) = P(\bar{v}(S))/P(\overline{u \cup v}(S)) = \sum_{v(S)} P(M(S)) / \sum_{(u \cup v)(S)} P(M(S) = \sum_{v(S)} \prod_{x \in C_{u \cup v}} l_x(S) / \sum_{(u \cup v)(S)} \prod_{y \in C_{u \cup v}} l_y(S) = g((u \cup B_{u \cup v})(S)).$$

$$(14.3)$$

This formula can be written in the form

$$P(v(S)) = g((u \cup B_{u \cup v})(S)) P((\overline{u \cup v})(S))$$

and by means of summation with respect to the spin states $\tilde{C}_{\nu}\cup_{\nu}(S)$ we obtain

Inserting (14.b) into (14.a) we finally find $g((u_{\omega v})(S)) = P((u \cup B_{\omega v})(S))/P(B_{\omega v}(S)) = P(u(S)|B_{\omega v}(S)). \quad (14.b)$

$$P(u(S)|(\overline{u \cup v}(S)) = P(u(S)|B_{u \cup v}(S)). \tag{15}$$

the whole residue of the lattice M but only on the states in the neighbourhood Thus the studied conditional probability does not depend on the state $(\overline{u \cup v})$ (S) on B_{uv} . In the case $v = \emptyset$ formula (15) implies

$$P(u(S)|\bar{u}(S) = P(u(S)|B_u(S)). \tag{16}$$

Let us have the following decomposition

$$M = a \cup b \cup \dots \cup u \cup v \tag{17.a}$$

of the lattice M where a, b, ..., u, v are mutually disjunct sets of lattice points.

$$P(M(S)) \equiv P(a(S)|\bar{a}(S)|P(b(S)|(\bar{a}\cup\bar{b})(S))...\times$$

$$\times P(u(S)(\bar{a}\cup\bar{b}...\cup\bar{u})(S))|P(v(S))|$$
(17.b)

Inserting the approximation (15) into the exact formula (17.b) we obtain

$$P(M(S)) = P(a(S)|B_a(S)) P(b(S)|B_{a\cup b}(S)) \dots$$

$$\cdots P(u(S)|B_{a \cup b \cdots \cup a}(S))P(v(S)). \tag{18}$$

equivalent forms of factorization (4), (11), (12). But this reduction is almost always form of the decomposition (17.a) since it always is reduced to the mutually the exact expression (17.b). The factorization (18) does not depend on the used contains conditional probabilities depending on much smaller clusters than those in Hence we see that in our approximative approach the factorized probability

> becomes obviously very quickly greater than the size of clusters from the set X. effectively applied. The size of the neighbourhoods occurring in the expression (18) special cases the factorization (18) is the same as the formula (12) which can be the problems connected with the calculation of $l_{\epsilon}(S)$, resp. q_{ϵ} . Only in a few very the theoretical one which is achieved by means of the formula (14.a). This is due to

fixed for all clusters $x \in X$. We use the following form of the decomposition (17.a) direction of the axis k_1 , i.e. $i = k_1 = k + 1$ where i is fixed for a given cluster and k is set X is chosen so that any cluster $x \in X$ lies in a layer with k+1 lattice points in the of a lattice point is described by the vector $(k_1, k_2, ..., k_d)$ where $k_1 = 1, ..., n$. The form of the factorization (18). Let us consider a d-dimensional lattice. A position A suitable choice of the decomposition (17.a) might sometimes lend to a useful

$$M = \bigcup_{i=1} a_i \tag{19.a}$$

$$a_i = \{k_1, k_2, ..., k_d\}; k_1 = i\},$$

i. e. the lattice M is decomposed into monoatomic layers in the direction of the axis k_i . Then the needed neighbourhoods are of the form

$$B_{a_1 \dots a_i} \subseteq a_{i+1} \cup \dots \cup a_{i+k}; i=1, \dots, n-k.$$
 (19.b)

expression (19.b). Such a casual enlargement of neighbourhoods might not make the approximation worse. Inserting (19.b) into (18) we obtain In what follows we will suppose that there is valid only the sign of equality in the

$$P(M(S)) = \prod_{i=1}^{n-k-1} P(a_i(S) (a_{i+1} \dots a_{i+k}) (S)) P(a_{n-k} \cup \dots \cup a_n) (S)) =$$

$$= \prod_{i=1}^{n-k} P(a_i \cup \dots \cup a_{i+k}) (S)) / \prod_{j=2}^{n-k} P((a_j \cup \dots \cup a_{j+k-1}) (S)).$$
(1)

This formula is convenient to apply in the calculations if the following condition is

$$a_i \cup a_{i+1} \cup \dots \cup a_{i+k} \in X; i = 1, \dots, n-k.$$
 (19.d)

euation (19.c) according to the axiom A_1 . Namely in this case we know all factors appearing on the right-hand side of the

set X contains all chains of k+1 neighbouring lattice points. Hence the formula (19.c) becomes as follows In the one-dimensional case the set a, is reduced to the ith lattice point and the

$$P(S_1, ..., S_n) = \prod_{i=1}^{n-k} P(S_i, ..., S_{i+k}) / \prod_{j=2}^{n-k} P(S_j, ..., S_{j+k-1}).$$
 (20)

All factors in this expression are known.

demonstrated by the following examples. the combersome calculation of $l_x(S)$, $x \in X$ or q_x , $z \in X'$. These problems will be (19.d) we do not know the factors occuring on the right-hand side of (19c) without not contain "a sufficient number" of convenient clusters "spread" over the whole lattice in the directions perpendicular to the axis k_i , in order to fulfil the condition If the lattice has no free ends in the direction of the axis k_1 or it the set X does

neighbours (i. e. k=1). Then the needed neighbourhoods are as follows Example 1.: Let us have a one-dimensional lattice. Its end points are nearest

$$B_{a \vee ... \vee a_i} = a_{i+1} \vee a_n, i=1, ... n-2$$

and from the formula (18) we have

$$P(s_1, ..., s_n) = \prod_{i=1}^{n-2} P(s_i, s_{i+1}, s_n) / \prod_{j=2}^{n-2} P(s_j, s_n).$$
 (21)

For instance in the simplest case of n=3 we obtain a cubic equation which is very There is not known any factor on the right-hand side of (21) according to axiom B.

points. Let the set X contain all pairs of nearest neighbours, i. e. $X = \{s_{11}, s_{12}\}, (s_{11}, s_{12}), (s_{11}, s_{12})\}$ s_{21}),}. The formula (18) then reads Example 2.: Let us have a two dimensional square lattice with 3 time lattice

$$P(s_{11}, ..., s_{33}) = P(s_{11}|s_{12}, s_{21}) (P(s_{12}|s_{13}, s_{21}, s_{22}) P(s_{13}|s_{21}, s_{22}, s_{23}) \times \times P(s_{21}, s_{22}, s_{23}, s_{31}) P(s_{22}|s_{23}, s_{31}, s_{32}) P(s_{23}|s_{31}, s_{32}, s_{33}) \times \times P(s_{31}|s_{32}, s_{33}) P(s_{22}, s_{33}).$$

$$(22)$$

cancels with the same term from the preceding factor according to the definition of the conditional probability. Thus it is necessary to solve 21 nonlinear equations Also in this formula we do not know directly any factor except the $P(s_{32}, s_{33})$, which

III. TEST OF FACTORIZATION

version of the Glauber model [17]. It is the linear kinetic Ising model without external field with transition probability Next we will test our factorization. For this purpose we use the exactly solvable

$$w(-s_i|s_i, s_{i-1}, s_{i+1}) \sim \frac{1}{2} \left[1 - \frac{1}{2} s_i(s_{i-1} + s_{i+1}) \right] \quad \gamma = \text{th } (2K)$$
 (23a)

Hamiltonian and equilibrium states equal to that of the corresponding Ising model with the

$$H = -K \sum_{i} s_{i} s_{i+1}. \tag{23b}$$

Its time development is given by the following system of kinetic equations

$$\frac{d}{dt} m(i) = -m(i) + \frac{1}{2} \gamma m(i-1) + \frac{1}{2} \gamma m(i+1)$$

$$\frac{d}{dt} m(i,j) = -2m(i,j) + \frac{1}{2} \gamma m(i-1,j) + \frac{1}{2} \gamma m(i+1,j) + \frac{1}{2} \gamma m(i,j-1) + \frac{1}{2} \gamma m(i,j+1) \dots,$$
(24)

where

$$m(i) = \langle s_i \rangle, m(i, j) = \langle s_i s_j \rangle.$$

$$m(i) = \langle s_{i} \rangle, \ m(i, j) = \langle s_{i} s_{j} \rangle.$$
The solution to this system is
$$m(i, t) = e^{-t} \sum_{n=-\infty}^{\infty} m(n; 0) I_{i-n}(\gamma t)$$

$$m(i, j, t) = m^{e}(i, j) +$$

$$e^{-2t} \sum_{p < r} m(p, r; 0) - m^{e}(p, r) I_{i-p}(\gamma t) I_{j-r}(\gamma t) -$$

$$- I_{i-r}(\gamma t) I_{j-p}(\gamma t) m^{e}(p, r) = R^{|p-r|}; \ R = \text{th } K,$$

$$(25)$$

where m'(p, r) is the equilibrium value of m(p, r, t) and $I_k(x)$ is the Bessel function of an imaginary argument. Supposing that the initial values are of the form

$$m(i;0) = m_0; m(i,j;0) = (R')^{|i-j|}; R' = \text{th } K',$$
 (26)

we obtain from (26)

$$m(i; t) = m_0 \exp \left[-(1 - \gamma)t \right]$$
 (27.a)

$$m(i, i+1; t \to +\infty) = R + \frac{2(\gamma' - \gamma)}{(1 - |\gamma|)(1 - |\gamma'|)} (4|\gamma|t)^{-3/2}$$
 (27.b)

$$\exp(-2(1-|\gamma|)\eta') = \text{th } (2K).$$

(27.c)

we will compare the exponent

$$\alpha_{\scriptscriptstyle m} = 2(1 - |\gamma|) \tag{28}$$

of the exact solution (26.c) with the corresponding exponent α_k of the approxima-

$$m_{12}^{(k)} = R + c_k \exp\left(-\alpha_k t\right)$$

obtained by means of the factorization (20) for given k. We assume translational invariance of the momenta, i. e.

$$m(i, j, ..., k) = m(1, j-i+1, ..., k-i+1)$$
 $i < j ... < k.$ (29)

m(i) = m(1), m(i, +i+1) = m(1, 2), ... (29.b)

The assumption (29) is justified namely for $t \to \infty$, i. e. in the neighbourhood of thermal equilibrium. The time development of this simplified model is given by the following equations

$$\frac{dm(1)}{dt} = (1 - \gamma) m(1)$$
 (30.a)

$$\frac{\mathrm{d}m(1,\,l+1)}{\mathrm{d}t} = -2m(1,\,l+1) + \gamma m(1,\,l) + \gamma m(1,\,l+2);\,m(1,\,1) = 1;$$

$$l = 1, 2, \dots$$
 (30.b)

The solution of (30.a) is exactly the same as that of (27.b).

The system (30.b) determines among other facts the exact form of m(1, 2). In order to obtain an approximation of m(1, 2) with the help of our factorization we consider first k equations of the system (30.b) for l = 1, ..., k. In this restricted system, there is only one undetermined quantity, namely m(1, k+2), which must be factorized. In our choice the set X contains all chains of k+1 mutualy neighbouring lattice points. The expansion of nonlinear factorization of momentum m(1, k+2) to the first order in deviations from equilibrium is as follows (Appendix)

$$m(1, k+2) = R^{k+1} - R^{2}[m(1, k) - R^{k-1}] + 2R[m(1, k+1) - R^{k}].$$
 (31)

By use of (30.b) for l = 1, ..., k and (31) we obtain

$$\frac{dx_1}{dt} = -2(1 - \gamma R)x_1 \text{ for } k = 1$$
 (32.a)

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = -2x_1 + \gamma x_2$$

$$\frac{dx_2}{dt} = \gamma x_1 - 2x_2 + \gamma x_3$$
 (32.b)

$$\frac{dx_{k-1}}{dt} = \gamma x_{k-2} - 2x_{k-1} + \gamma x_k$$

$$\frac{\mathrm{d}x_k}{\mathrm{d}t} = \gamma(1-R^2)x_{k-1} - 2(1-\gamma R)x_k; \quad k=2,3,...$$

$$x_1 = m(1, l+1) - m^{\circ}(1, l+1; m^{\circ}(1, l+1) = R'.$$
 (32.c)

Now, we can easily find the following exponents α_k for k=1, 2, 3

$$\alpha_1 = 2(1-R) = 2\sqrt{1-\gamma^2}$$

$$\alpha_2 = 2 - \gamma R - |\gamma| = 1 - |\gamma| + \sqrt{1 - \gamma^2}$$

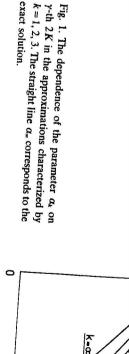
 $\alpha_3 = 2 - \frac{1}{2} \gamma R - |\gamma| \sqrt{\frac{1}{4}} r^2 + 2$

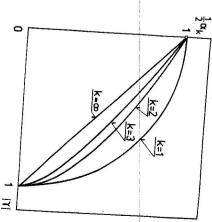
(33)

$$\alpha_{\infty} = 2(1-|\gamma|)$$

$$\alpha_1 \geqq \alpha_2 \geqq \alpha_3 \geqq \alpha_*$$

where the equalities hold only it $_{\gamma}=0$ or $|\gamma|=1$ (see Fig. 1). We can infer from the form of the equations (32.b) and from the ineguality (33) that the exponents α_k converge to the exact value α_{∞} with an increase of k i. e. with increase of size of clusters contained in the set X.





IV. CONCLUSION

As has been shown, the studied factorization is actually convenient to apply only in the one-dimensional case. According to the formula (22) our factorization means the following approximation of the conditional probability

$$P(s_i|s_{i+1},...,s_{i+k},s_{i+k+1},...) = P(s_i|s_{i+1},...,s_{i+k})$$

(34)

in the one-dimensional case

An intuitively understandable and dimension independent result is the correspondence between the two following aspects of the problem. The first aspect is the Hamiltonian of the equilibrium counterpart of the studied kinetic model and the

$$-kTH(t) = \sum_{z \in X} q_z(t) \prod_{i \in z} s_i.$$
(35)

type of the spin interaction. into the probabilities of states on spatially separated clusters regarding the given dimension. There ought to be added some further physical requirements to be built evidently not sufficient to determine an applicable factorization in more than one Axioms A, B, and C and the requirement of a correct thermal equilibrium are

suggestions and helpful discussions Concluding I should like to express my gratitude to Dr. Anton Surda for valuable

the nearest smaller clusters is given as follows The factorization of the momentum m(j, j+p) with respect to the momenta on

$$m(j,j+p) = \sum_{s_{j-\dots,s_{j+p}}} s_j s_{j+p} P(s_j, \dots, s_{j+p-1}) P(s_{j+1}, \dots, s_{j+p}) / P(s_{j+1}, \dots, s_{j+p-1}), \quad (A1)$$

order in the deviations means of formula (6). We have to expand the nonlinear quantity (A1) to the first where the probabilities on the right-hand side are expressed through momenta by

$$x_{i,j...} = m(i, j, ...) - m^{e}(i, j, ...)$$
 (A2)

to find the following equilibrium probabilities calculated by means of the transfer matrix method [16]. This method also allows us of momenta from their equilibrium values. The equilibrium values are easily

$$P^{\bullet}(s_{i}, ..., s_{i}) = \frac{1}{2}(2 \cosh K)^{-(j-i+1)} \exp \left(K(s_{i}s_{i+1} + ... + s_{j-1}s_{i})\right) \quad (j > i). \quad (A3)$$

The wanted expansion is of the following form

$$x_{i,j+p} = \sum_{i=1}^{3} \sum_{z \in M_i} \left(\frac{\partial m(j,j+1)}{\partial m_z} \right) e^{X_z}$$
 (A4a)

where

$$M_{1} = \{z | z = \{j\} \cup v, \quad v \in C\}$$

$$M_{2} = \{z | z = \{j + p\} \cup v, \quad v \in V\}$$

$$M_{3} = V = \{v | v \subseteq \{j + 1, ..., j + p - 1\}\}.$$
(A4b)

With the help of (A1), (A3), (A4) and the formula

$$\frac{\partial}{\partial m_i} P(s_i, ..., s_j) = 2^{-(j-i+1)} \prod_{l \in I} s_{li}, \tag{A5}$$

if $z \subseteq \{i, ..., j\}$, otherwise = 0

which is the consequence of the expression (6), we have

$$\left(\frac{\partial m(j,j+p)}{\partial m_z}\right)_{e,z\in M_1} = R \text{ if } z = \{j,j+p-1\}$$

=0 othervise

$$\left(\frac{\partial m(j,j+p)}{\partial m_z}\right)_{c, z \in M_2} = R \text{ if } z = \{j+1, j+p\}$$

= othervise

(A6)

$$\left(\frac{m(j,j+p)}{\partial m_z}\right)_{c, z \in M_3} = -R^2 \text{ if } z = \{j+1, j+p-1\}$$

=0 othervise

Thus we obtain

$$x_{i,\,j+p} = R^2 x_{j+1,j+p-1} + R(x_{i,\,j+p+1} + x_{j+1,\,j+p}) \quad (x_{i,\,j} = 0)$$
he case of translational:

and in the case of translational invariance

$$x_{1, p+1} = -R^2 x_{1, p-1} + 2R x_{1, p} \quad (x_{1, 1} = 0).$$

8

REFERENCES

- [1] Balescu, R.: Equilibrium and Nonequilibrium Statistical Mechanics, John Wiley and Sons, New

- [2] Roberts, J. K.: Proc. Roy. Soc. A 161 (1937), 141.
 [3] Roberts, J. K.: Proc. Roy. Soc. 152 (1935), 445.
 [4] Kawasaki, K.: Phys. Rev. 145 (1966), 224.
 [5] Matsudaira, N.: J. Phys. Soc. Japan 23 (1967), 232.
 [6] Matsudaira, N.: Can. J. Phys. 45 (1967), 2091.

- [7] Kawasaki, K.: in Phase Transitions and Critical Phenomena, Vol. 2, Eds.: C. Domb, M. S. Green, Academic Press, London, 1972.
 [8] Bowker, M., King, D. A.: Surface Sci. 71 (1978), 583, Surface Sci. 72 (1978), 208.

- [9] Leuthäusser, V.: Z. Phys. B 37(1980), 65.
 [10] Mazenko, G. F., Hirsch, J. E., Nolan, M. J., Valls, O. T.: Phys. Rev. Lett. 44(1980), 1083.
 [11] Mazenko, G. F., Valle, O. T.: Phys. Rev. B 24(1981), 1404.
 [12] Mazenko, G. F., Nolan, M. J., Freedman, R.: Phys. Rev. B 18(1978), 2281.
 [13] Safran, S. A., Sahni, P. S., Grest, G. S.: Phys. Rev. B 28(1983), 2693.
 [14] Hendlay, Ch. L.: Phys. Rev. Lett. 54(1985), 1030.

- [15] Kaski, K., Ala-Nissilä, T., Guton, J. D.: Phys. Rev. B 31 (1985), 310.
 [16] Baxter, R. J.: Exactly Solved Models in Statistical Mechanics, Acad. Press, London, 1982. [17] Glauber, P. J.: Math. Phys. 4 (1963), 249.

Received March 3rd, 1986