THE EXACT SOLUTION OF THE LINEAR ISING MODEL WITH FIRST AND SECOND NEAREST-NEIGHBOUR INTERACTIONS

BRANISLAV MAMOJKA*, Bratislava

This article presents an exact solution of the linear Ising model with first and second nearest-neighbour interactions. The thermodynamical functions are expressed by their dependence on the temperature as well as on the ratio of the interaction energies. There is also determined the temperature for the extreme of the heat capacity and the dependence of this extreme on the ratio of the interaction energies.

I. INTRODUCTION

interaction and an arbitrary number of neighbours. This, is however, a very retical point of view to investigate the linear Ising model with the general of interacting potential, therefore, it appears to be interesting from the theoall the existing linear Ising models there is a restriction on the specific type sition for long range interactions of the form $J(n) = Jn^{-\alpha}$, if $1 < \alpha < 2$ [5]. In of Katz [4] who calculated the thermodynamical function of the linear Ising has shown that the linear one-dimensional Ising model can indeed have a tranmodel with the interaction potential of the form $\gamma \exp \{-\gamma | i-j|\}$. Dyson of the further neighbours in a linear constellation. Well-known is the model of the original Ising model consists in taking into account the interactions -neighbour two-dimensional Ising models [3]. Another way of the extension Since the Onsager results there have been a number of studies of the secondmodel for a square lattice of spins with nearest-neighbour interactions [2]. famous formula for the free energy per particle of the two dimensional Ising model have been proposed and calculated. In 1944, Onsager presented his Since that time, many various modifications and extensions of the Ising of a one dimensional lattice with only the nearest-neighbour interactions. us to understand phase transitions is the Ising model proposed in 1925 [1]. Ising originally calculated the statistical partition function only for the case The well-known example of idealized statistical model systems which help

complicated problem. This is why we have been dealing with the linear Isingmodel with the general potential but only with first and second nearest-neighbour interactions.

The exact solution of the linear Ising model with first and second nearest neighbour interactions enables us to obtain besides the temperature dependence of thermodynamical functions also their dependence on the ratio of this interaction energies and, mainly, to evaluate the temperature of the extreme of the heat capacity and value of this extreme as the function of the above mentioned ratio. The solution is obtained by the diagramatic method generally used in statistical physics.

II. THE DESCRIPTION OF THE MODEI

The linear Ising model with first and second nearest-neighbour interactions and free ends is described by the following Hamiltonian

$$H = E_1 \sum_{k=1}^{N-1} \sigma_k \sigma_{k+1} + E_2 \sum_{l=1}^{N-2} \sigma_l \sigma_{l+2}, \tag{1}$$

where E_1 and E_2 are the interaction energies between first and second nearest neighbours, respectively, and σ_k are the Pauli matrices.

The partition function is given by the well-known formula

$$Z = \text{Tr} \left[\exp \left(-H/kT \right) \right]. \tag{2a}$$

Denoting

$$a=-E_1/kT$$
 $r=E_2/E_1$
 $u= h(a)$
 $v= h(r\cdot a)$

3

and applying the equation generally valid for the Pauli matrices

$$\exp(x \cdot \sigma_k \sigma_l) = \operatorname{ch} x + \sigma_k \sigma_1 \cdot \operatorname{sh} x,$$

we obtain for the partition function

$$Z = (\operatorname{ch} a)^{N-1} (\operatorname{ch} (r \cdot a))^{N-2} \operatorname{Tr} \left[\prod_{k=1}^{N-1} (1 + \sigma_k \sigma_{k+1} \cdot u) \prod_{l=1}^{N-2} (1 + \sigma_l \sigma_{l+2} \cdot v) \right].$$
 (2b)

In the square brackets of the preceding formula there is a sum of the terms which represent the products of the Pauli matrices and powers of functions u and v. As it is known, the trace of any term of this sum containing at least one odd power of any Pauli matrix equals zero. After tracing the formula (2b) the nonzero terms consist of the factor 2^N multiplied by a product of the

^{*} Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta, 899 30 BRA-TISLAVA, Czechoslovakia.

powers of the function u and v. The former factor is caused by tracing over the powers of the Pauli matrices which are unit matrices and the latter factor will be evaluated by the diagramatic method. Then the partition function can be written as

$$Z_N = 2^N (\operatorname{ch} a)^{N-1} (\operatorname{chr} \cdot a)^{N-2} (1 + T_N),$$
 (2c)

where T_N is the sum of the contributions of all so-called allowed diagrams, e.g. non-zero ones, constructed on an N-site linear lattice with free ends. These diagrams are constructed as follows: The Pauli matrices refer to the vertices, first nearest-neighbour interactions refer to the lines with the weight factor u and the second nearest-neighbour interactions refer to the line with the weight factor v.

Any allowed diagram must obey the following conditions: (i) In any lattice site there can only meet, 0, 2, or 4 lines. (This follows from taking into account first and second nearest neighbour interactions and from the fact that the trace of odd power of the Pauli matrix is zero). (ii) All diagrams are closed, e.g. they have no free ends. (This follows from property 1 as well). (iii) All lines of any diagram are simple. (This is a consequence of formula (2b)).

For further considerations it is convenient to define the following concepts: If any two arbitrary vertices of a diagram are connected by its lines, the diagram is called the connected one. (see Fig. 1).



Fig. 1. Example of a connected diagram.

If in any vertex of a connected diagram there meet just two lines, the diagram is called the simple one (see Fig. 2).

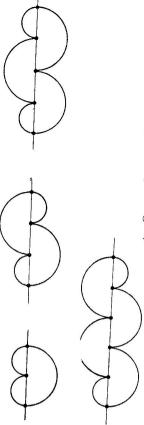
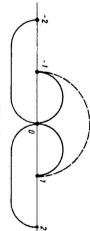


Fig. 2. Examples of simple diagrams.

We will show that any connected diagram can be expanded into simple diagrams which are independent of each other. To do this it is sufficient to prove the following assertion. By an arbitrary vertex in which four lines meet it is possible to divide any connected diagram into two parts without crossing any line. By the symbol O we denote the vertex in which four lines meet and those on its right or left by the numbers $1, 2, \ldots$, or by the numbers $-1, -2, \ldots$, respectively. In order to prove our statement it is necessary to show that the line of the type v, connecting the vertices -1 and 1, is not allowed (see Fig. 3). We cannot take into account other lines connecting vertices located on the right-hand side of the vertex O with vertices located on its left-hand side, since we have only lines of the types u and v. According symmetry of our problem it is sufficient to study diagrams in one direction from the vertex O, e. g. in the direction pointing to the right.



Tig. 3

We shall prove whether it is possible to extend the diagram (see Fig. 3) in accordance with the above mentioned conditions valid for the allowed diagrams, i.e. whether its contribution might be non-zero.

A) Suppose the diagram continues in the vertex 1. Then it must continue by two lines pointing to the right, one of them (of the type u) ends in the vertex 2 and the other (of the type v) ends in the vertex 3. In this case, however, the vertex 2 (as to the structure) is equivalent to the vertex 1 of the original diagram and the vertex 3 to the vertex 2 of the original diagram. If the diagram continues in the vertex 2 as well, we have the same situation as above. (The possibility that the diagram does not continue in the vertex in question or in another vertex equivalent to it will be treated in the case B). This procedure can be continued up to the vertex preceding the last one. If in this vertex the diagram does not continue, there ends only one line in the last vertex, and according to the above mentioned properties of the allowed diagrams, the contribution of the studied diagram equals zero. If in the vertex preceding the last one the diagram continues, three lines must meet in this vertex and the contribution of this diagram is equal to zero again.

B) Suppose the diagram does not continue in the vertex 1. Eventually, the diagram, studied under item A, does not continue in the vertex equivalent to the vertex 1, then it must continue in the vertex 2 by one line. If this line

contribution is equal to zero. by one line, or, in one of the internal vertices, three lines meet so that its u gives the case A). Thus it is clear that also in case B the diagram must end k+1 to k+3 (connection of vertices k+2 and k+3 by the line of type of the type u from the vertex k+2 to k+1, and by the line of type v from of the type v from the vertex k to the vertex k+2, then by means of the line combined with the following situation: 2. The diagram continues by the line us to the foregoing consideration of the case B. This structure can be also bution is equal to zero) or continue by a simple line: the latter case has led dealing with, might either end by the diagram of the type A (then its contritype v) would be equivalent to the vertex O (see Fig. 3). The diagram, we are under the case A, begins so that this vertex (the end vertex of the line of the 1. In the vertex, in which the line of the type v ends the diagram, studied the diagram continues by the line of the type v, then there can arise two cases: is equal to zero. If, however, in the vertex 2 or in another following vertex, vertee, where only one line ends and, therefore, the contribution of this diagram By means of the constant use of the lines of the type u, we arrive at the last is of the type u, the diagram must also coninue in the vertex 6 by one line

From the above considerations it follows that in all possible cases the contribution of the diagram with the line of the type v, connecting vertices 1 and -1, equals 0 (i.e. the line of the type v connecting vertices 1 and -1 is not allowed) if four lines meet in vertex O. Thus our statement has been proved. From what has been said so far there follows also a method of the division of the connected diagram into simple diagrams. Any connected and allowed diagram can be divided into simple diagrams performing the division in all the vertices in which four lines meet. Then the contribution of a connected diagram is given by the product of the contribution of the simple diagrams

Let us now prove that there exists only one simple diagram O_k $(k \ge 3)$ constructed over k neighbouring sites on a linear lattice with free ends and evaluate its contribution.

According to condition (iii) two lines meet in the end vertices of any simple diagram — one of the type u and one of the type v. Because of this fact there must exist two branches of the diagram (built up from lines u and v) connecting its end vertices. These branches do not coincide in any internal vertex of the diagram. Their coincidence in the internal vertex causes that the diagram becomes a non-simple one (there meet four lines). If we permit that the above-mentioned branch contains an internal line of the type u, the branches must coincide, since we have only the lines of the type u connecting first nearest-neighbour vertices and lines of the type v connecting second nearest-neighbour vertices. Thus, the second branch can by no way pass the line of the type u

involved in the first branch without its concidence with the first branch in at least, one of the vertices connected by the internal line u. As a consequence of this, the line of the type u cannot be the internal line of any of the two branches. The branches which do not coincide in any internal vertex can be built up only in one way, i.e. when all internal lines are of the type v. This show that there exists only one allowed simple digram O_k constructed on k neighbouring sites of a linear lattice, whose contribution can be easily evaluated being

$$O_k = u^2 v^{k-2}$$
 $k = 3, 4, \dots$ (4)
 $O_0 = O_1 = O_2 = 0.$

(Then also $T_k = 0, k = 0, 1, 2, \dots$ From what has been said so far it follows that there is only one way of the expansion of the alowed connected diagram into allowed simple ones.

Using our knowledge of the structure of the allowed diagrams we can find a recurrent formula for T_N . Suppose we know all T_k $k=3,\ldots,N-1$. A linear lattice with N sites can be built up from the lattice with N-1 sites by adding the N-th site. Then T_N on the lattice constructed in this way contains

$$T_{N-1}$$
, (5a)

all simple diagrams whose end vertex is located on the N-th site of the lattice

$$\sum_{k=3}^{N} O_k \tag{5b}$$

and all diagrams (except that of 5(b)) containing as a part a simple diagram whose end vertex is located on the N-th site of the lattice

$$\sum_{k=3}^{N-2} O_{N-k+1} T_k.$$
 (5c)

By the summation of all contributions (5) we obtain for T_N

$$T_N = T_{N-1} + \sum_{k=3}^{N-2} O_{N-k+1} T_k + \sum_{k=3}^{N} O_k \qquad N = 5, \dots$$
 (6)

Adding to Eq. (6) that for T_{N-1} multiplied by -v and using the relation $O_k = vO_{k+1}$, which follows from Eq. (4), we have

$$T_N - (1+v)T_{N-1} + (v-u^2v)T_{N-2} = u^2v$$
 $N = 5, \dots$ (7)
 $T_4 - (1+v)T_3 = u^2v$
 $T_3 = u^2v$
 $T_2 = T_1 = T_0 = 0$.

 T_N is given by the solution of the system (7) of N-2 nonhomogeneous linear equations by means of the Crammer rule. The determinant of this system is equal to 1. Thus, T_N is given by the determinant of the system (7), where the first column is replaced by the right-hand sides of Eq. (7). Expanding this determinant, we get

$$T_N = u^2 v \left[\sum_{k=1}^{N-3} (-1)^k D_k + 1 \right], \tag{8a}$$

where D_k is the determinant of the k-th degree. Its elements occurring above, below and on the diagonal line are the numbers $v - vu^2$, 1 and -1 - v, respectively. The other elements are identically equal to 0. Expanding the determinant D_k , we obtain the following recurrent formula

$$D_N + (1+v)D_{N-1} + (v-u^2v)D_{N-2} = 0, (9)$$

the solution of which is (see Appendix (A8), (A9))

$$D_N = (X^{N+1} - Y^{N+1})/(X - Y) \qquad N = 0, 1, \dots$$

$$D_0 = 1,$$
(10)

where D_0 is introduced consistently with our problem and has been defined only for convenience.

$$X = -1/2(1+v) + [1/4(1+v)^2 - v(1-u^2)]^{1/2}$$

$$Y = -1/2(1+v) - [1/4(1+v)^2 - v(1-u^2)]^{1/2}.$$
(11)

According to (10) the formula (8a) may be rewritten

$$T_N = u^2 v \sum_{k=0}^{N-3} (-1)^k D_k.$$
 (8b)

Inserting (10) into (8b) we have

$$T_N = u^2 v(X - Y)^{-1} \{ [1 - (-Y)^{N-1}]/(1 + Y) - [1 - (-X)^{N-1}]/(1 + X) \},$$
(12a)

which becomes after a simple modification

$$T_N = -1 + (X - Y)^{-1}[(1 + X)(-Y)^{N-1} - (1 + Y)(-X)^{N-1}].$$
(12b)

Thus, from (2c) and (12b) we get the partition function

$$Z_N = 2^{N}(\operatorname{ch} a)^{N-1}(\operatorname{ch} ra)^{N-2}(X - Y)^{N-1}[(1 + X)(-Y)^{N-1} - (1 + Y)(-X)^{N-1}]$$

$$N = 3, \dots$$
(13)

Since -Y is a sum of two non-negative values (the expression under the sign of the square root is always non-negative for all physically allowed values

a nd-X is the difference of the same two non-negative values) we have |X| < |Y|. The case of |X| = |Y| is possible only if u = 1 and v = -1. (The case u = 0 and v = 1 is non-physical). It occurs when $T \to 0$ and $E_2 > 0$. We need not take this case into account since, from the physical point of view, we can always reach the zero temperature from the higher one, for which there holds |X| < |Y|. In our model, where further than second nearest-neighbour interactions are neglected, the problem of the stability of the system when $E_2 > 0$, becomes very complicated.

III. THE THERMODYNAMICS OF OUR ISING MODEL

Thermodynamical functions will be calculated from the partition function per spin defined as follows

$$\ln Z = \lim_{N \to \infty} [(\ln Z_N)/N], \tag{14}$$

the form of which is (when using the properties of the parameters Y and X) the following

$$Z = 2(\operatorname{ch}a)(\operatorname{chr}a)(-Y) = (\operatorname{ch}a)(\operatorname{chr}a)\{1 + v + [(1+v)^2 - 4v(1-u^2)]^{1/2}\}.$$
 (15)

The thermodynamical functions of the linear Ising model with first and second nearest-neighbour interactions evaluated according to (15) will be compared with the thermodynamical functions of the linear Ising model with first nearest neighbour interactions to which there belongs the partition function ([6] E. Montroll: Lekcii po modeli Isinga, formula (3, 6)

$$Z = 2cha. (16)$$

If the parameter r=0, the partition function (15) passes into the partition function (16) and the thermodynamical functions calculated from (15) are equal to those calculated from (16).

The thermodynamical functions will be calculated after the well-known formulas [7]:

(i) Free energy

$$F = -kT \ln Z = E_1 a^{-1} \ln Z. \tag{17a}$$

(ii) Energy

$$E = kT^2 \frac{\mathrm{d} \ln Z}{\mathrm{d}T} = E_1 \frac{\mathrm{d} \ln Z}{\mathrm{d}a} . \tag{18a}$$

(iii) Entropy

$$S = \frac{E - F}{T} = -\frac{\mathrm{d}F}{\mathrm{d}T} = k \left(\ln Z - a \frac{\mathrm{d} \ln Z}{\mathrm{d}a} \right). \tag{19a}$$

(iv) Heat capacity

$$C = \frac{\mathrm{d}E}{\mathrm{d}T} = ka^2 - \frac{\mathrm{d}^2 \ln Z}{\mathrm{d}a^2} \ . \tag{20a}$$

By the evaluation of the thermodynamical functions at $T \to 0$, it is convenient to use the parameter

$$P = -4v(1+v)^{-2}(1-u^2) = [\exp(-4ra) - 1](cha)^{-2}.$$
 (21a)

If $T \to 0$, we get

$$P \to 0 \quad \text{if } E_2 < \frac{1}{2}|E_1|$$
 (21b)
 $P \to 4 \quad \text{if } E_2 = \frac{1}{2}|E_1|$
 $P^{-1} \to 0 \text{ if } E_2 > \frac{1}{2}|E_1|$.

According to (17a) the free energy is

$$F = E_{1}a^{-1}\ln\left(\cosh(a)\cosh(ra)\right) + E_{1}a^{-1}\ln\left\{1 + v + [(1 + v)^{2} - 4v(1 - u^{2})]^{1/2}\right\},$$

$$F \to -|E_{1}| + E_{2} \text{ if } E_{2} \leqslant \frac{1}{2}|E_{1}| \text{ and } T \to 0$$

$$F \to -E_{2} \text{ if } E_{2} \leqslant \frac{1}{2}|E_{1}| \text{ and } T \to 0$$

$$F \to -kT \ln 2 \text{ if } T \to \infty$$

and for r=0

$$F = -\mathbf{k}T \ln (2\mathbf{ch}a)$$
 (17c)
 $F \to -|E_1|$ for $T \to 0$
 $F \to -\mathbf{k}T \ln 2$ for $T \to \infty$.

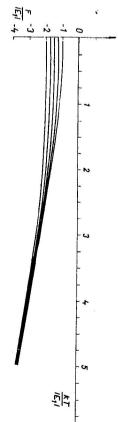


Fig. 4. The temperature dependence $kT/|E_1|$ of the thermodynamic potential $F/|E_1|$ for values of the parameter $\tau' = -E_2/|E_1| = 0$; 0.25; 0.50; 0.75; 1, to which the curves beginning from the top of the figure refer, respectively.

The temperature dependence of the free energy is a monotonically decreasing function. In Fig. 4 we see the plot of the function $F/|E_1|$ for the value of the parameters

$$r' = -\frac{E_2}{|E_1|} = 0$$
; 0.25: 0.50; 0.75; 1
$$0 \leqslant \frac{kT}{|E_1|} \leqslant 5$$
.

(22)

In limiting case, we have

$$\frac{F}{|E_1|} \to -1 - r' \quad \text{for} \quad T \to 0. \tag{17d}$$

By means of (18a) we get for the energy

$$\frac{E}{E_{1}} = \frac{1}{2} r v^{-1} (1 + v^{2}) + \left[u - \frac{1}{2} r v^{-1} (I - v)^{2} \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v^{-1} (1 - v^{2}) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - \frac{1}{2} v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v^{2} \right) \right] (1 + v) \left[(1 + v)^{2} - v \left(1 - v$$

and for r=0

$$E = E_1 u$$

$$E \to -|E_1| \text{ for } T \to 0$$

$$E \to 0 \text{ for } T \to \infty.$$
(18c)

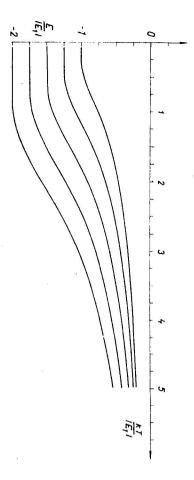


Fig. 5. The temperature dependence $kT/|E_1|$ of the energy E/E_1 for the values of the parameter $r' = -E_2/|E_1| = 0$; 0.25; 0.50; 0.75; 1, to which the curves beginning from the top of the figure refer, respectively.

As expected, the energy monotonically increases with increasing temperature. In Fig. 5 we see the plot of the function E/E_1 for the parameters (22), for which it is valid

$$\frac{E}{|E_1|} \to -1 - r' \quad \text{for } T \to 0$$

$$\frac{E}{|E_1|} \to -r' \quad \text{for } T \to \infty.$$
(18d)

From the formula (19a) we obtain the entropy

$$\frac{S}{k} = \ln \left(\operatorname{cha \, chra} \right) + \ln \left\{ (1+v) + \left[(1+v)^2 - 4v(1-u^2) \right]^{1/2} \right\} - \frac{1}{2} rav^{-1} (1+v^2) - a \left[u - \frac{1}{2} rv^{-1} (1-v)^2 \right] (1+v) \left[(1+v)^2 - 4v(1-u^2) \right] \right\} - \frac{1}{2} rav^{-1} (1+v)^2 - \frac{1}{2} rav^{-1} (1+v)^2$$

and for r = 0 it turns out to be

$$rac{S}{k} = \ln (2 ext{ch} a) - a u$$
 $S o 0 \ T o 0$
 $S o k \ln 2 \ T o \infty$.

(19c)

The entropy increases again with the increasing temperature and its temperature dependence for the parameters (22) is plotted in Fig. 6. The heat capacity

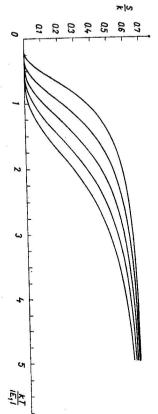


Fig. 6. The temperature dependence $kT/|E_1|$ of the entropy S/k for the same values of the parameter r'=0;0.25;0.50;0.75;1, as in the foregoing pictures and in the same sequence beginning from above.

is defined by the formula (20a) as follows

$$k^{-1}a^{-2}C = -\frac{1}{2}r^{2}v^{-2}(1+v)^{2}(1-v)^{2} + [(1+4ru)(1-u^{2}) \times (1-v)^{2}(1+v) + \frac{1}{2}r^{2}v^{-2}(1-v)^{2}(1+v)^{5} - r^{2}(1-u^{2})v^{-1}(1-v)^{2}(1+v)(3v^{2}+2v+3)] \times [(1+v)^{2}-4v(1-u^{2})]^{-3/2} \times [(1+v)^{2}-4v(1-u^{2})]^{-3/2}$$

$$C \to 0 \quad T \to 0$$

$$C \to 0 \quad T \to 0$$

$$C \to 0 \quad T \to \infty$$
(20b)

and for r = 0 we have

$$\frac{C}{k} = a^2(\mathrm{ch}a)^{-2}$$

 $C \rightarrow 0$, it must have at least one positive extreme. Since the heat capacity is non-negative observable and for $T \to 0$ and $T \to \infty$

 $r'=-E_2/|E|$ for $0\leqslant r'\leqslant 1$, i.e. for the non-positive E_2 . In Fig. 7 there is plotted the dependence of C/k on the temperature for the parameters (22). The temperature at which this extreme is reached in the dependence of paramete In Tab. 1 the values of the extreme are given as well as the values of the

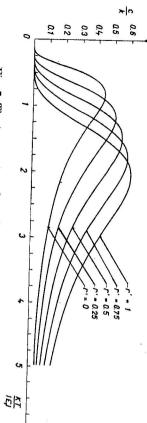
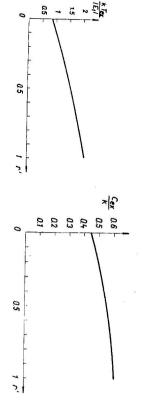


Fig. 7. The temperature dependence of the heat capacity C/k

the heat capacity on r', for r' from 0 to 1 is shown in Fig. 9. 0 to 1 is plotted in Fig. 8 and the dependence of the value of the extreme of dependence of the temperature for the extreme of the heat capacity on r' from

for the above-mentioned reasons as well as for the fact that the factor Thermodynamical functions for r' < 0, i.e. $E_2 > 0$ have not been evaluated

$$[(1+v)^2-4v(1-u^2)]^{1/2},$$



capacity on the parameter $r' = -E_2/|E_1|$. $kT_{ex}/|E_1|$, of the maximum of the heat value of the heat capacity C_{ex}/k on the Fig. 8. The dependence of the temperature. Fig. 9. The dependence of the extremum parameter $r' = -E_2/|E_1|$.

in the numerical calculations. for r' < 0 and $T \approx 0$ becomes very small, which causes great complications

IV. CONCLUSIONS

From what has been said so far it follows that:

- on the expected temperature increase (more exact the increase of the quantity value of r' increases). of these maximal values on the second interaction energy (for $E_2 < 0$ the $kT/|E_1|$) by which the heat capacity reaches its maximum and the dependence -neighbour interactions. The most important result consists in the confirmation interactions has many similar features to that with the linear first nearest-(i) The extended linear Ising model with first and second nearest-neighbour
- behaviour of our Ising model mainly in the low temperature region. (ii) The second nearest-neighbour interaction affects the thermodynamic
- neighbours. said long-range linear Ising models, since their potentials are either only the first and second neighbours have opposite signs. This is impossible by the so it can describe a physical situation whereby the interaction energies between ly in the fact that the interaction energies can possess both $\operatorname{signs}(+\operatorname{and}-)$ and linear Ising model with the general interaction by taking into account further positive or negative. It would be, therefore, worthwhile to investigate the [6], mentioned in Introduction, the significance of our model consists especia-(iii) In comparison with the linear Ising model with long range ineractions

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The extreme of the heat capacity

	nand Sloboda, member of the computer laboratory.	work I wish to thank RNDr. Ferdi-	preparing the final version of the ma-	veral other colleagues for their help in	the manuscript. I am indebted also to	my attention to some or the quadratic terature, as well as for the reading of	for helpful discussions and for drawing	de to RNDr. Vladimír Majerník, CSc.	I should like to express my gratitu-
0.900 0.950 1.000	0.790 0.800 0.850	0.650 0.700	0.550 0.550	0.450	0.350	0.200	0.100 0.150	0.000 0.050	$r^{\prime}=-E_{1}/ E_{2} $
1.965 2.020 2.073	1.855	1.686 1.743	1.569	1.449	1.324	1.127 1.194	0.986 0.058	0.834 0.912	$kT/ E_1 $
0.598 0.603 0.607	0.588	0.571 0.577 0.583	0.565	0.543 0.551	0.526	0.494 0.505	0.469 0.482	$0.439 \\ 0.455$	Clk

$$D_n + aD_{n-1} + bD_{n-2} = 0,$$

(A1)

can be solved in the following way: [9]

Let us find the values X and Y satisfying the condition:

$$D_n - XD_{n-1} = Y(D_{n-1} - XD_{n-2})$$

$$D_n - YD_{n-1} = X(D_{n-1} - YD_{n-2})$$

(A2)

Eqs. (A2) can be rerwritten as

$$D_n - XD_{n-1} = Y^{n-2}(D_2 - XD_1), (A3a)$$

$$D_n - YD_{n-1} = X^{n-2}(D_2 - YD_1), (A3b)$$

from where we get

$$a = -X - Y$$

$$b = XY. (A4a)$$

The parameters a and b solve the quadratic equation:

$$q^2 + aq + b = 0. (A4b)$$

we get Multiplying Eq. (A3a) by Y and substracting it from (A3b) multiplied by X,

$$D_n = (X - Y)^{-1} [X^{n-1}(D_2 - YD_1) - Y^{n-1}(D_2 - XD_1)].$$
 (A5)

If X = Y, Eqs. (A3) reduce to the equation

$$D_n - XD_{n-1} = X^{n-2}(D_2 - XD_1). (A6)$$

It implies

$$D_n = X^{n-2}[(n-1)D_2 - (n-2)XD_1]. \tag{A7}$$

In our case Eqs. (9), (A1) and (A4a) give

$$X = -\frac{1}{2}(1+v) + \left[\frac{1}{4}(1+v)^2 - v(1-u^2)\right]^{1/2}$$

$$Y = -\frac{1}{2}(1+v) - \left[\frac{1}{4}(1+v)^2 - v(1-u^2)\right]^{1/2}.$$
(A8)

96

Because of

$$D_1 = -1 - v = X + Y$$
 $D_2 = (1 + v)^2 - v(1 - u^2) = X^2 + XY + Y^2$

the expression for D turns out to be finally

$$D_{n} = (X^{n+1} - Y^{n+1})(X - Y)^{-1}$$

$$n = 0, 1, \dots$$

$$D_{0} = 1.$$
(A9)

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