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CALCULATION OF THE FREE ENERGY OF ISING SYSTEMS BY A RECURSION METHOD

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A new recursion method is proposed for the calculation of the thermodynamics of Ising-spin models with short range interaction. The method is exact in one dimensions, while for higher dimensions a truncation scheme is developed. The approach is tested in the two-dimensional Ising model. The results are within 0.7% of the exact reduced free energy per spin.

1. Introduction

In recent years much work has been done on different applications of the real space renormalization transformations, introduced first by Niemeijer and van Leeuwen[1]).

The real space renormalization transformations are simple and clear realizations of the original ideas of Kadanoff[2]) in the context of the powerful formalism worked out by Wilson[3]). The construction of approximate renormalization equations for the coupling constants is based on well-known methods of statistical mechanics, like the cumulant and the cluster expansion[1,4]) and the variational approach[5]). In spite of some uncertainty on the nature of perturbation schemes[6,7]), it was found that the cumulant and the cluster methods are very successful in two dimensions and yield acceptable results also in three dimensions[7,8,10]). The variational approach is very accurate in all dimensions of physical interest[9]).

The renormalization transformations are able to give us not only the fixed points, the critical exponents and the cross-over behaviour of the system but, as pointed out by Nienhuis and Nauenberg[4]), can also be used for the calculation of the free energy, even far from the critical region.

A different method, based on the functional recursion relation between the partition functions of spin cells of different size with fixed boundary conditions was introduced by Berezinskii in the context of the $X-Y$ model and was applied by Migdal to gauge fields[18]). Later Kadanoff reformulated this recursion method in terms of standard renormalization transformations[19]).

In this paper a simple real space recursion relation method is presented, based on the successive summation of surface spins of a semi-infinite lattice. Although the basic idea is the same as in renormalization theory, namely the reduction of an infinite number of degrees of freedom to a number tractable in a computer, the elimination of degrees of freedom is not accompanied by a scale change of the lattice constant. This means that critical parameters cannot be determined directly but only through the analysis of the free energy.

The general formulation of the recursion relations is illustrated in the case of the one-dimensional Ising model with external field and it is shown that the method is exact in one dimension. For higher dimensions a systematic approach is introduced for the truncation of the infinite set of recursion equations. This truncation scheme becomes exact at high temperatures and is tested in this paper on the two-dimensional Ising model. Six successive approximations are calculated and the sixth approximation is within 2% of the exact result at the critical point (the high temperature results are converted to the low temperature region with the help of the dual transformation, so the poorest results are obtained at the critical point). The successive approximations form a function progression which tends monotonically from below to the Onsager solution[17]). Using an appropriate extrapolation method the results can be improved to differ less than 0.7% from the exact reduced free energy per spin. It is also shown that this method can be easily extended to models where spins have more than two states.

2. General formulation of recursion equations

Consider a general hamiltonian[1]):

$$H(\{s_i\}) = \sum_{a \in L} K_a \prod_{i \in a} S_i, \tag{1}$$

where L is a d-dimensional semi-infinite lattice having a spin $s_i = \pm 1$ at every lattice point, a and K_a denote some special types of sublattices and the related coupling constants (including the $\beta = -1/k_B T$ factor), respectively.

The statistical mechanical calculation of the thermodynamics of the model (1) is found by analysing the asymptotical behaviour of the canonical partition function:

$$Z_N(K_a) = \sum_{\{s_i\}_{i=1}^{N}} \exp H(\{s_i\}), \tag{2}$$

for $N \to \infty$. One possibility is to study how the progression

$$Z_2/Z_1,\ Z_3/Z_2, \ldots, Z_N/Z_{N-1}, \ldots \to \lambda, \tag{3}$$

goes to $\lambda = \exp(-F/k_B TN)$, where F is the free energy of the system.

It seems reasonable to say that $N \approx 25$–30 is the practical limit of a direct calculation. Of course there are many perturbational[16]), variational[20]) and Monte Carlo methods[11]) to determine Z_N. However, these methods generally fail when many length scales play an equally important role, as e.g. in the critical region.

The renormalization group transformations have the advantage of essentially reducing the number of length scales. From a practical point of view, renormalization is a very convenient method to handle the problem of large N, based on the observation that transforming an N-variable hamiltonian to an N'-variable hamiltonian ($N' < N$) of the same structure reduces the number of configurations by a factor $2^{(N-N')}$. By the iteration of this transformation the calculation of the (critical) properties of the system is reduced to the calculation of the properties of only a small number of neighbouring spins forming the so-called "block-spin cell".

The method to be followed here works essentially in the same way. Let us cut our d-dimensional semi-infinite lattice in layers of $(d-1)$ dimension in the same manner as in the transfer matrix theory[15]). The main requirement is that the interaction between layers has to be a nearest neighbour interaction:

$$H^{(1)} = \sum_{j=1}^{\infty} H_j + \sum_{j=1}^{\infty} H_{j,j+1}, \tag{4}$$

where the j index labels the layers and the upper index of H equals to the starting value of j. The partition function (2) can be rewritten as the sum over the spins of the first $\{s_i^{(1)}\}$, second $\{s_i^{(2)}\}$, etc. layers:

$$Z = \sum_{\{s_i^{(1)}\}} \sum_{\{s_i^{(2)}\}} \cdots \exp H^{(1)}. \tag{5}$$

We choose the layers to be parallel to the free surface of the semi-infinite lattice and we number them starting with the surface layer. If now we sum over the spins of the first (surface) layer, we obtain a positive function of the spins $\{s_i^{(2)}\}$ lying on the second layer:

$$Z = \sum_{\{s_i^{(2)}\}\{s_i^{(3)}\}} \sum \cdots \Psi(\{s_i^{(2)}\}) \exp H^{(2)}, \tag{6}$$

This function can be exponentiated as

$$\Psi(\{s_i^{(2)}\}) = \exp[\Phi(\{s_i^{(2)}\})], \tag{7}$$

where the $\Phi(\{s_i^{(2)}\})$ function can be expanded in terms of the orthogonal basis consisting of all possible products of spins $s_i^{(2)}$:

$$\begin{aligned}\Phi(\{s_i^{(2)}\}) &= A_0 + \sum_i A_i s_i^{(2)} + \sum_{j>i} A_{ij} s_i^{(2)} s_j^{(2)} + \cdots \\ &= \sum_n \left(\sum_{\alpha_1} \sum_{\alpha_2 > \alpha_1} \cdots \sum_{\alpha_n > \alpha_{n-1}} A_{\alpha_1 \alpha_2 \ldots \alpha_n} s_{\alpha_1}^{(2)} s_{\alpha_2}^{(2)} \ldots s_{\alpha_n}^{(2)} \right).\end{aligned} \tag{8}$$

Apart from the generated constant term A_0, the hamiltonian is renormalized to

$$\tilde{H}^{(2)} = H^{(2)} + \Phi(\{s_i^{(2)}\}) - A_0. \tag{9}$$

This means that every possible coupling is generated between the spins of the second layer, which actually forms the surface layer. The number of such couplings equals the total number of configurations of a layer. The next step is to sum up every spin of the second layer $\{s_i^{(2)}\}$. This results in the renormalization of all the surface intralayer coupling constants for which a set of recursions can be written. Note that the renormalization is restricted to the layer actually forming the surface by the condition that between layers only nearest neighbour interaction acts. This interlayer interaction is not affected by the renormalization process and ensures that the recursion equations have fixed points at all. Therefore, after a sufficient number of iterations the surface coupling constants will reach their fixed points. The reduced free energy per spin,

$$f(K_a) \equiv -F/k_B TN - \ln 2$$

is obtained from the fixed point value of the generated constant coupling (3):

$$f(K_a) = A^*(K_a)/N^{d-1} - \ln 2. \tag{10}$$

One advantage of such a formulation is that the generation of new coupling constants is restricted to a $(d-1)$-dimensional subspace of the lattice. From the above formulation it is also clear that an iteration step does not change the scale of the lattice constant, as in the usual renormalization theory, where the lattice is homogeneously dilated at every iteration.

In the next section it will be shown that this method is exact for one-dimensional Ising systems with short range interaction. In dimensions higher than one some approximation is needed to make tractable the large number of recursion relations. Fortunately, several methods have been worked out to this end in the real space renormalization theory. We use a high temperature truncation scheme, which is the generalization of an idea of Wilson[13]). This approach is based on the use of a generalized decimation transformation[5]), more exactly on a general star–poligon transformation[14]) (in fact the decimation transformation applied to a square lattice is a star–square transformation).

3. One-dimensional Ising spin models

Let us start with a semi-infinite chain of $\frac{1}{2}$ Ising spins:

$$H^{(1)} = K \sum_{j=1}^{\infty} s_j s_{j+1} + h \sum_{j=1}^{\infty} s_j, \tag{11}$$

where the upper index of H is again equal to the starting value of j. Now the layers are formed by the individual spins, the interaction between layers is

nothing but the interaction between spins and the external field is the only contribution to the intra-layer energy.

Following our method we sum up the first (surface) spin, then

$$Z = 2 \sum_{\{s_i\}_{i=2}^{\infty}} \cosh(Ks_2 + h) \exp H^{(2)}, \tag{12}$$

and the resulting $\cosh(Ks_2 + h)$ function depends, as expected, on s_2. Exponentiating this function we get

$$\cosh(Ks_2 + h) = \exp(A + Bs_2), \tag{13}$$

where A and B can be determined since (13) has to be true for every value of s_2:

$$A(K, h) = \tfrac{1}{2} \ln[\cosh(K + h) \cosh(K - h)], \tag{14a}$$

$$B(K, h) = \tfrac{1}{2} \ln[\cosh(K + h)/\cosh(K - h)]. \tag{14b}$$

The hamiltonian looks now as

$$\tilde{H}^{(2)} = H_{(2)} + Bs_2 = Ks_2 s_3 + (h + B)s_2 + H^{(3)} \tag{15}$$

apart from the generated constant $A - \ln 2$. Therefore, after N summations the surface external field obeys the following recursion relation:

$$h_N = h + B(K, h_{N-1}), \tag{16}$$

with $h_1 = h$. Observe that $A(K, h_N)$ just equals $\ln(Z_N/2Z_{N-1})$ and according to (3) tends to $f(K, h)$ for large N. Therefore, if one wants to know the reduced free energy per spin, $f(K, h)$, with an arbitrary small ϵ accuracy, the iteration of (16) has to be continued until $|h_N - h_{N-1}| < \epsilon$, which means that $|A(K, h_N) - A(K, h_{N-1})| < \epsilon$.

Of course the fixed point equation for the surface external field:

$$h^* = h + B(K, h^*)$$

can be solved analytically. If we put the resulting expression into (14a), we obtain the expected result[12]):

$$A(K, h^*(K, h)) = \ln \tfrac{1}{2}\{e^K \cosh h + [e^{2K} \sinh^2 h + e^{-2K}]^{1/2}\}. \tag{17}$$

The generalization of this method to other one-dimensional $\frac{1}{2}$ Ising models is straightforward. For example, the model

$$H^{(1)} = \sum_{j=1}^{\infty} (hs_j + Ks_j s_{j+1} + Ls_j s_{j+2} + Ms_j s_{j+1} s_{j+2}) \tag{18}$$

can be solved by iterating the recursions

$$h_N = h + B(h_{N-1}, K_{N-1}, L, M) + C(h_{N-2}, K_{N-2}, L, M), \tag{19a}$$

$$K_N = K + D(h_{N-1}, K_{N-1}, L, M), \tag{19b}$$

with $h_0 = K_0 = 0$, $h_1 = h$, $K_1 = K$ and

$$B(h, K, L, M) = \tfrac{1}{4} \ln[\cosh \alpha \cosh \beta / \cosh \gamma \cosh \delta], \tag{20a}$$

$$C(h, K, L, M) = \tfrac{1}{4} \ln[\cosh \alpha \cosh \gamma / \cosh \beta \cosh \delta], \tag{20b}$$

$$D(h, K, L, M) = \tfrac{1}{4} \ln[\cosh \alpha \cosh \delta / \cosh \beta \cosh \gamma], \tag{20c}$$

where

$$\alpha = h + K + L + M, \qquad \beta = h + K - L - M,$$

$$\gamma = h - K + L - M, \qquad \delta = h - K - L + M.$$

The fixed point values of h_N and K_N obtained from (19) are then substituted into

$$f = A(h^*, K^*, L, M) = \tfrac{1}{4} \ln[\cosh \alpha \cosh \beta \cosh \gamma \cosh \delta]. \tag{20d}$$

We finish the treatment of the one-dimensional $\frac{1}{2}$ Ising-spin models with two remarks. First, the restriction to short range interaction is due to practical considerations: too many independent coupling constants greatly increase the number of points where the free energy has to be computed; on the other hand an interaction range longer than 8–10 lattice constants leads to a slow exponentiation operation. Secondly, let us remark that the whole procedure can be generalized to models where the spins have more than two states, for example a model like (11), with $s_i = -1, 0, +1$. In this case a possible orthogonal basis is $\{1, s_i, 3s_i^2 - 2\}$ and the exponentiation has to be done accordingly.

4. A truncation scheme – test in the two-dimensional Ising model

In dimensions higher than one, the surface layer has many spins and we have to solve in a practical way an infinite set of recursion equations. To this end a truncation scheme will be introduced in the context of the two-dimensional Ising model on a square lattice. The reason of such a choice is obvious: (a) the method can be tested by comparing it with the exact Onsager solution[17]) and (b) the generalization of this approach to other models and higher dimensions is evident.

Before going into the details of the calculation let us introduce some notations. The lattice points of the square lattice will be denoted by (x, y), where this means the xth lattice point of the yth row. At the same time we will use a "moving" denotation (more convenient to write the iteration equations) namely the spin to be summed up in the next step will be denoted by zero and the spins coupled to it will be numbered from 1 to N_s. Every coupling between these spins has different names before ($K_{\alpha_1 \alpha_2 \ldots \alpha_n}$) and after ($A_{\alpha_1 \alpha_2 \ldots \alpha_n}$) the summation over the zeroth spin.

The layers are formed by the rows of the lattice and one starts by summing the (1, 1) spin, as shown in fig. 1a. Now K_{01} and K_{02} equals the original nearest neighbour coupling, $K = J/k_B T$. The iteration transformation[14]) ($N_s = 2$) of

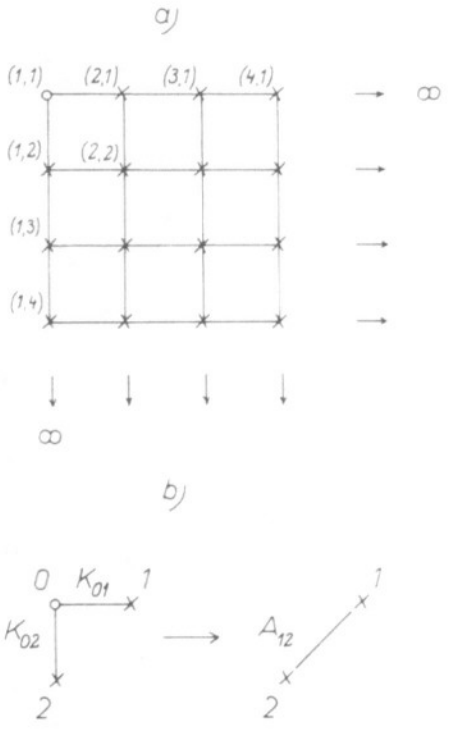


Fig. 1. (a) The semi-infinite square lattice before the summation of (1, 1) spin; (b) the iteration transformation ($N_s = 2$).

fig. 1b generates a constant term A_0 and an A_{12} coupling between the (2, 1) and the (1, 2) spin:

$$A_0 = \tfrac{1}{2} \ln[\cosh(K_{01} + K_{02}) \cosh(K_{01} - K_{02})], \tag{21a}$$

$$A_{12} = \tfrac{1}{2} \ln[\cosh(K_{01} + K_{02})/\cosh(K_{01} - K_{02})]. \tag{21b}$$

The (2, 1) spin now has three coupled neighbours, as shown in fig. 2a. After converting the A_{12} coupling in K_{03}, the (2, 1) spin is summed up by the star–triangle ($N_s = 3$) transformation shown in fig. 2b and yields the new couplings:

$$A_0 = \tfrac{1}{4} \ln[\cosh \alpha \cosh \beta \cosh \gamma \cosh \delta], \tag{22a}$$

$$A_{12} = = \tfrac{1}{4} \ln[\cosh \alpha \cosh \delta/\cosh \beta \cosh \gamma], \tag{22b}$$

$$A_{13} = \tfrac{1}{4} \ln[\cosh \alpha \cosh \gamma/\cosh \beta \cosh \delta], \tag{22c}$$

$$A_{23} = \tfrac{1}{4} \ln[\cosh \alpha \cosh \beta/\cosh \gamma \cosh \delta], \tag{22d}$$

where

$$\alpha = +K_{01} + K_{02} + K_{03}, \qquad \beta = -K_{01} + K_{02} + K_{03},$$

$$\gamma = +K_{01} - K_{02} + K_{03}, \qquad \delta = +K_{01} + K_{02} - K_{03}.$$

Numerical values of these couplings are summarized in table I, together with values obtained after performing the next step, described by fig. 2c. Analysing these values two facts can be remarked. First, a generated coupling has a

TABLE I

Numerical values of coupling constants generated by the summation of the first, second and third spin of the first row.

Transformation of	Generated coupling constants	$K = 0.10$	$K = 0.44$	$K = 1.00$	$K = 10.0$
Fig. 1b					
$K_{01} = K_{02} = K$	$A_0 = A_{12}$	0.00993	0.17280	0.66250	9.65343
Fig. 2b	A'_0	0.00998	0.18398	0.77383	14.1336
$K_{01} = K_{02} = K$	A'_{12}	0.00993	0.16912	0.56877	5.1733
$K_{03} = A_{12}$	$A'_{13} = A'_{23}$	0.00098	0.06073	0.31581	4.8267
Fig. 2c	A''_0	0.00998	0.18487	0.76681	11.9949
$K_{01} = K_{02} = K$	A''_{12}	0.00993	0.16885	0.57656	7.3120
$K_{03} = A'_{12}$	$A''_{13} = A''_{23}$	0.00098	0.05934	0.26965	2.5866
$K_{04} = A'_{13}$	$A''_{14} = A''_{24}$	0.00010	0.02113	0.14791	2.4133
	A''_{34}	0.00001	0.00767	0.08733	2.3120
	A''_{1234}	-0.2×10^{-6}	−0.00249	−0.07126	−2.3120

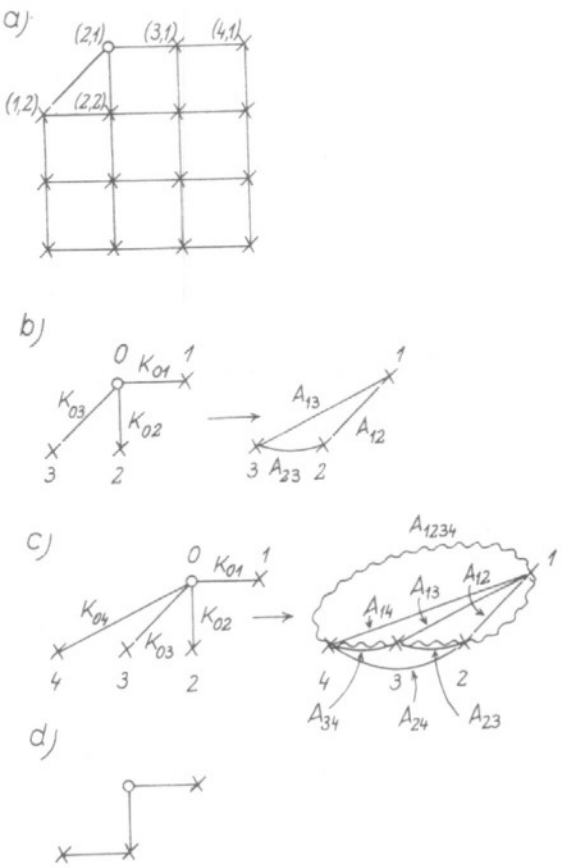


Fig. 2. (a) The lattice after the summation of the (1, 1) spin; (b) the star–triangle transformation ($N_s = 3$); (c) the star-square transformation ($N_s = 4$); (d) the shifting figure of the first approximation.

smaller absolute value if it is connecting a larger number of spins. Secondly, between two coupling constants connecting an equal number of spins, those which are closer to the spin on the right and the spin below the zeroth spin are larger. As can be seen from table I the difference between these coupling constants increases when $K \to 0$.

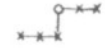
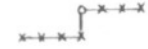
The above observations are the background for our truncation scheme, which works as follows. In the lowest order we stop at the situation shown in fig. 2b, and before doing the transformation of fig. 2c we simply neglect the A_{13} coupling compared with A_{12}. Therefore, the number of neighbours of the (3, 1) spin is reduced back to $N_s = 3$ and the same (22) star–triangle transformation has to be repeated, with $K_{01} = K_{02} = K$, $K_{03} = A_{12}$. Dropping the coupling A_{13}, after every summation, we shift to right the figure shown in fig. 2d, which is accordingly called the shifting figure of the approximation. The shifting figure contains the maximal number of spins connected together, taken into account exactly before applying the truncation. We repeat this shift until the difference between K_{03} and the generated coupling A_{12} is within a given small ϵ. As in the one-dimensional case, we can argue that in such a way virtually the whole first row has been summed up, because the summation of further spins does not change the value of generated constants (22). We can say that the coupling constants A_0, A_{12} and A_{23} have reached their first row fixed points, $A_0^{*(1)}$, $A_{12}^{*(1)}$ and $A_{23}^{*(1)}$, respectively. Note that only the couplings connecting spins of the first (upper) and the second (lower) row, as e.g. the A_{12} coupling, play an active role in this shifting process. We call these couplings active couplings constants to distinguish them from the renormalized surface couplings, as e.g. the A_{23} coupling. The same procedure is repeated for the second row, with $K_{02} = K$ and $K_{01} = K + A_{23}^{*(1)}$. (This means that before starting the summation of the second row we cut out from the lattice the first columns necessary for A_{23} to reach its fix point.) The iteration is done until the value of the renormalized surface nearest neighbour coupling differs by no more than ϵ in two successive rows, i.e. $|A_{23}^{*(k+1)} - A_{23}^{*(k)}| < \epsilon$. Then, the reduced free energy per spin just equals the $(k+1)$th row fixed point value of the generated constant, $A_0^{*(k+1)}$ [see eqs. (3), (10) and (22)]. Note that the value of the nearest neighbour interaction between layers K_{02} remains equal to the original K during the whole iteration process and in fact ensures that we get fixed points at all.

From table I it is expected that this truncation scheme is better for smaller K, when the difference between A_{12} and A_{13} is really important. Table II contains some of our numerical results for different orders of approximation, represented by their shifting figures. It can be seen that the first order approximation described here is almost exact for $K \leq 0.1$, is within 2.5% at $K = 0.3$, and within 10% of the exact result at the critical point, $K_c = \text{th}^{-1}(\sqrt{2} - 1) = 0.44069$. Taking into account that the square lattice is self-dual, i.e. the reduced free energy per spin transforms like

$$f(K^*) = f(K) + \tfrac{1}{2} \ln \frac{\sinh 2K^*}{\sinh 2K} \tag{23}$$

TABLE II

Reduced free energy per spin functions obtained from successive approximations up to sixth order

K							Extrapolation	Onsager solution
0.05	0.002505	0.002505	0.002505	0.002505	0.002505	0.002505	0.002505	0.002505
0.10	0.01008	0.01008	0.01008	0.01008	0.01008	0.01008	0.01008	0.01008
0.15	0.02290	0.02292	0.02293	0.02293	0.02293	0.02293	0.02293	0.02293
0.20	0.04121	0.04130	0.04137	0.04138	0.04138	0.04138	0.04138	0.04138
0.25	0.06527	0.06560	0.06588	0.06593	0.06595	0.06596	0.06596	0.06596
0.30	0.09525	0.09620	0.09706	0.09724	0.09735	0.09738	0.09740	0.09741
0.35	0.1312	0.1334	0.1355	0.1361	0.1365	0.1367	0.1369	0.1369
0.386[a]	0.1606	0.1642	0.1679	0.1691	0.1701	0.1705	0.1711	0.1712
0.40	0.1728	0.1771	0.1816	0.1832	0.1845	0.1851	0.1861	0.1862
0.431[b]	0.2017	0.2080	0.2146	0.2174	0.2196	0.2208	0.2231	0.2242
0.44	0.2099	0.2167	0.2240	0.2271	0.2297	0.2312	0.2344	0.2359
0.45	0.2196	0.2272	0.2353	0.2390	0.2420	0.2437	0.2478	0.2504
0.45 *	0.2279	0.2342	0.2410	0.2436	0.2457	0.2470	0.2493	
0.50	0.2710	0.2831	0.2962	0.3029	0.3088		0.3271	0.3327
0.50 *	0.3220	0.3256	0.3293	0.3305	0.3315	0.3319	0.3325	

[a] Dual pair of $K = 0.50$ [eq. (24)].

[b] Dual pair of $K = 0.45$.

* Obtained with the help of the dual transformation (23).

when the coupling constant is changed to

$$K^* = -\tfrac{1}{2} \ln \operatorname{th} K, \tag{24}$$

all the results obtained for $K < K_c$ can be converted to the $K > K_c$ region. Therefore, in lowest order the approximate free energy is within 10%, which is a quite good result taking into account the extreme simplicity of this approximation.

In the second order calculation the (3, 1) spin is also exactly summed up by the star–square ($N_s = 4$) transformation shown in fig. 2c. Then, every active coupling connecting the fourth spin to the first spin, namely A_{14} and A_{1234} is dropped after every shift. After the summation of the kth row, the surface nearest neighbour coupling K_{01} is renormalized to $K + A_{23}^{*(k)} + A_{34}^{*(k)}$.

Such a calculation was done up to sixth order ($N_s = 8$). In the sixth order approximation 35 active coupling constants and four surface coupling constants were renormalized. The star–octagon transformation needed at every shift consists of 128 equations, solved numerically (the time necessary to this end was about 8 s in a CDC 3300 computer). The reduced free energy per spin is within 2% of the exact result.

Moreover, as can be seen from table II, the functions corresponding to the successive orders of approximations form a progression, which tends monotonically from below to the Onsager solution. Writing out the differences of subsequent orders at fixed K, it appears that these numbers go to zero like an exponential function. Using an exponential curve fit program (HP-65 Stat. Pac. 1-23A) the results can also be extrapolated to the value displayed in table II. The extrapolated function is within 0.7% of the exact solution; note that the free energy per spin itself is within 0.2%!

Of course the results for the internal energy $\partial f/\partial K$ and for the heat capacity $K^2(\partial^2 f/\partial K^2)$ are poorer due to the inaccuracy of the numerical derivation operation. The computing time necessary to obtain the results of table II with an $\epsilon = 10^{-5}$ accuracy was about 45 min in a CDC 3300 computer.

Although this method works as expected from the physical intuition and the experience of real space renormalization transformations, there are many unanswered questions concerning the mathematical foundation of such an approach. For example, the author was not able to prove that every order of the truncation scheme presented here yields to a function which is below the exact free energy, as can be conjectured from results obtained up to sixth order.

Since for $N_s \geq 5$ two or more shifting figures can be constructed, as shown in fig. 3 for $N_s = 7$, one has to motivate the choice of table II. As can be seen from the corresponding shifting figures, in the first case (fig. 3a) only the nearest neighbour surface coupling is renormalized ($K_{01} = K + A_{23}^* + A_{34}^* + A_{45}^* + A_{56}^* + A_{67}^*$), while in the second case (fig. 3b) also the second neighbour coupling ($K_{01} = K + A_{34}^* + A_{45}^* + A_{56}^* + A_{67}^*$ and $K_{02} = A_{35}^* + A_{46}^* + A_{57}^*$) and in the third case (fig. 3c) the third neighbour and the four spin couplings are renormalized, too ($K_{01} = K + A_{45}^* + A_{56}^* + A_{67}^*$, $K_{02} = A_{46}^* + A_{57}^*$ and $K_{03} = A_{47}^*$,

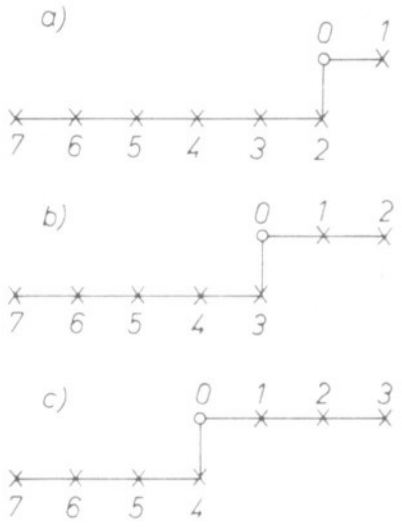


Fig. 3. The three possible shifting figures for $N_s = 7$.

$K_{0123} = A^{*}_{4567}$). The results for this three approximations are summarized in table III. The approximation shown in fig. 3c gives the best results because the successive contributions to a given surface coupling constants are steeply decreasing, $A_{23} > A_{34} > A_{45} \ldots$, so it is better to take into account a further coupling constant than to calculate a new correction term to the old coupling constants, as say K_{01} (in fact $A_{24} > A_{34}$, $A_{25} > A_{45} \ldots$). Therefore, the best shifting figure for a given N_s contains nearly the same number of spins on the upper as on the lower row, taking into account as many different coupling constants as possible.

A more delicate question concerns the nature of the approximations shown in table II. One can argue, for example, that in the first order approximation described above, A_{13} is of the same order of magnitude as A_{23} and is not consistent to drop only A_{13}.

A "consistent" approach would require that we take into account only the coupling constants which are at least of the same order as the largest coupling

TABLE III
Results of the approximations represented by the shifting figures of fig. 3

K	Fig. 3a	Fig. 3b	Fig. 3c
0.05	0.002505	0.002505	0.002505
0.10	0.01008	0.01008	0.01008
0.15	0.02292	0.02293	0.02293
0.20	0.04131	0.04138	0.04138
0.25	0.06562	0.06593	0.06595
0.30	0.09628	0.09728	0.09735
0.35	0.1336	0.1363	0.1365
0.40	0.1777	0.1840	0.1845
0.45	0.2283	0.2415	0.2420

dropped at every shift. An example of such an approximation is the second order truncation ($N_s = 4$) with $K_{01} = K + A^*_{23}$. From table IV one can see that the results obtained in this way are only slightly better than the "inconsistent" first order approximation of table II. In fact, this truncation scheme is surely not a simple perturbation theory, where the different orders of magnitude can be easily identified. In high order truncations it happens that many coupling constants differ only by a factor of two or less and there is not a well-defined criterion to decide which ones have to be dropped and which not. The final argument in favour of the pragmatic approach used in the calculation of different order truncations of table II (namely that every coupling constant compatible with a given shifting figure was taken into account, independently of its order of magnitude), is that the computing time increases by a factor of four when N_s increases by 1. Together with the appropriate choice of the shifting figure this approach leads to the best results which can be obtained for a given N_s.

5. Concluding remarks

In this paper we have presented a very simple recursion method for the numerical evaluation of the thermodynamics of Ising-spin systems. This method is exact in one dimension and gives very good results in the two-dimensional Ising model, where a truncation approach is used. One main advantage of this method is that the renormalization process is restricted to a $(d-1)$-dimensional subspace of the lattice. The main difference between our method and the usual renormalization theory is that during the iteration of recursion relations the lattice constant is not changed.

The investigation of other models seems also to be possible. The most natural application of this method is, however, the calculation of surface

TABLE IV
Comparison of the first consistent approximation with the first and second order results

K		First order consistent	
0.10	0.01008	0.01008	0.01008
0.20	0.04121	0.04124	0.04130
0.25	0.06527	0.06537	0.06560
0.30	0.09525	0.09553	0.09620
0.35	0.1312	0.1318	0.1334
0.40	0.1728	0.1739	0.1771
0.45	0.2196	0.2215	0.2272

properties. To this end we have only to collect the free energy results after the summation of each layer.

The truncation scheme presented here becomes exact at high temperatures. It is desirable to work out a truncation scheme also for the low temperature region because many of the models of physical interest have no dual lattices. Further work is also needed for a better understanding of the error introduced by the truncation method, in order to develop a variational approach improving further the (accuracy/computing time) ratio.

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