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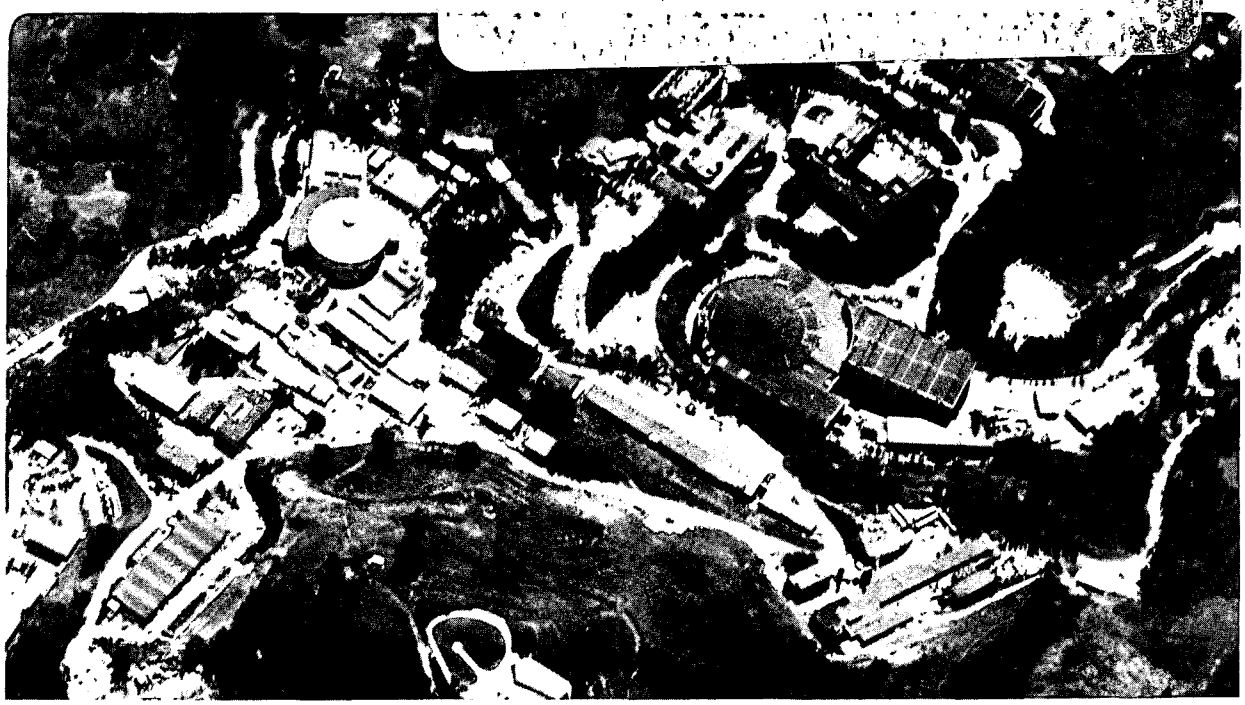

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A FAMILY OF METHODS FOR THE SOLUTION OF LATTICE MODELS[1]

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ABSTRACT

A family of methods for evaluating the thermodynamic functions for a class of lattice models that includes the Ising model is discussed. The family of methods is characterized by successive increases in the lattice size followed by extrapolation. It is shown that the usual transfer matrix method is a member of the family and the best member of this family is found. We are also concerned with the further acceleration of these methods. For this reason on the basis of the member of this family which is related to the transfer matrix method an extra linear extrapolation algorithm is presented. By this algorithm, not only the bulk physical quantities can be evaluated more precisely but also an approximation to the boundary thermodynamic quantities can be obtained. A new expression for the boundary free energy of the Ising model is derived. In addition, the convergence to the thermodynamic limit for the scaling method which has been presented by Chorin is shown. Some numerical results for the bulk and boundary thermodynamic functions of the Ising model are included

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1. Introduction

The goal of this paper is to consider a family of methods for evaluating the partition function, the free energy and other thermodynamic quantities for a class of lattice models that includes the Ising model. The family of methods is characterized by successive increases in the lattice size followed by extrapolation. All methods in this family are related to the linkage algorithm [10]. One member of this family is the usual transfer matrix method [22]. Another member of this family is the particular factored solution used in [10]. One aim of the present paper is to find the best member of this family. We are also concerned with the further acceleration of these methods. An extra linear extrapolation algorithm which generalizes methods used in conjunction with the transfer matrix method will be presented. In addition, the scaling algorithm [10] which uses a spin batch to accelerate the convergence to the thermodynamic limit will be discussed.

In [10], several methods for reducing the amount of labor required for the evaluation of the thermodynamic functions for lattice methods were presented. Among these methods the basic one is the linkage algorithm which relates the partition function and the free energy of a union of blocks to the same quantities evaluated on the component blocks. This linkage algorithm leads to an exact and fast enumeration scheme that reduces drastically the labor required for evaluating the partition function of a finite lattice (for L Ising spin in the plane the amount of labor is reduced from $O(2^L)$ to $2^{O(\sqrt{L}+\log_2 L)}$). The linkage algorithm allows us to add spin locations to a given spin configuration and compute the thermodynamic quantities for the augmented configuration at a small cost. On the basis of the linkage algorithm two other methods which

accelerate the rate at which quantities evaluated on a finite lattice converge to their thermodynamic limits were presented in [10]. One was called a factored solution. Chorin showed that for Ising spins on a line the thermodynamic limit was reached by the factored solution. For a two-dimensional Ising model the numerical results showed that this algorithm accelerates the convergence. The other method was "scaling" which further accelerates the convergence of the factored solution. In [10] there was only a heuristic justification for the method and the numerical results provided were only for one lattice size which was not sufficient to show the convergence to the thermodynamic limit.

The present paper is based on [10]. First, it will be demonstrated that from the linkage algorithm a family of methods can be derived and the usual transfer matrix method can be related to this family. It will be shown that the particular factored solution used in [10] is the best in this family. Second, for the member of this family which is related to the transfer matrix method, an extra linear extrapolation algorithm will be presented. We add the word "extra" because an extrapolation has already been included in the original method. By this algorithm, not only the bulk physical quantities can be evaluated more precisely but also an approximation to the boundary quantities can be obtained at the same time. Along the line of the algorithm a new expression for the boundary free energy of Ising model will be derived. Third, some numerical results which show that when the lattice size increases, the thermodynamic functions computed by the scaling and the extra linear extrapolation algorithm converge to their thermodynamic limits will be included. Then a review of the particular factored solution, the scaling method and the extra linear extrapolation algorithm will be given.

In order to accelerate the convergence of finite-lattice sequences to their bulk limits, various extrapolation methods have been considered by a number of authors. In fact, the analysis of numerical finite-lattice data by finite-size scaling theory is essentially an extrapolation [4]. In connexion with this theory, a computationally important development is the phenomenological renormalization presented by Nightingale [18]. After that in [14] a sequence transformation method has been used to extrapolate the bulk critical parameter from the data for finite lattices with

periodic boundary condition. These methods have yielded some accurate results. In the present paper, we still discuss the extrapolation. However, we do not start with finite-size scaling. Without consideration of all finite-size effects, we only pay attention to the effect due to the "dangling bonds" at the boundary [23]. Our extrapolation process is equivalent to eliminating this boundary effect from bulk thermodynamic quantities computed for a finite system. The extrapolation algorithm considers the finite lattice with non-periodic boundary conditions, by which both the bulk and the boundary thermodynamic functions can be studied.

For simplicity, we shall concentrate on the two-dimensional Ising model with free edges. Both bulk and boundary thermodynamic functions will be computed. Our numerical results are consistent with the theoretical predictions and comparable with the results in [12] [17] [18] [20]. The numerical results for boundary thermodynamic quantities are given here apparently for the first time. The two-dimensional Ising model is discussed as an illustration. All of these methods can be applied to more complicated lattice systems and can be used in conjunction with some other methods, for example, Monte-Carlo methods.

This paper is organized as follows. In section 2 we briefly describe the Ising model and some relevant theoretical results. In section 3 we discuss the family of methods which are derived from the linkage algorithm followed by extrapolation. In section 4 an extra linear extrapolation algorithm is given. In section 5 we present computational results. Finally, in section 6 We use the finite-size scaling theory to estimate the critical point.

In this paper we do not discuss the estimates of critical exponents. This work will be done in another article.

2. Problem and Notation

We briefly describe the ferromagnetic Ising model and some relevant theoretical results.

Consider an $m \times n$ rectangular lattice with sites (i,j), $1 \leq i \leq m$, $1 \leq j \leq n$, carrying spin $\mu_{i,j}$, $\mu_{i,j} = \pm 1$. A set of possible values $\mu = \left\{ \mu_{i,j} \right\}$ is called a configuration. The energy of a configuration, in appropriate units, is

$$E(\mu) = -\sum_{i=1}^{i=m-1}\sum_{j=1}^{j=n}\mu_{i,j}\mu_{i+1,j} - \sum_{i=1}^{i=m}\sum_{j=1}^{j=n-1}\mu_{i,j}\mu_{i,j+1}. \tag{2.1}$$

The partition function is

$$Z_{m\times n} = \sum_{\{\mu\}}\exp(-zE(\mu)), \tag{2.2}$$

where $z = \frac{1}{T}$ and T is the temperature. The free energy $\phi_{m\times n}$ per spin for the finite lattice is

$$\phi_{m\times n} = (m\times n)^{-1}\log Z_{m\times n}, \tag{2.3}$$

and the bulk free energy per spin in the thermodynamic limit is

$$\phi = \lim_{m,n\to\infty}\phi_{m\times n}. \tag{2.4}$$

The bulk internal energy U is

$$U = -\frac{\partial\phi}{\partial z}, \tag{2.5}$$

and the bulk specific heat C is

$$C = z^2\frac{\partial U}{\partial z}. \tag{2.6}$$

In the Ising model a critical point z_c, i.e. a non-analytic point of ϕ, is found, $\sinh(z_c) = 1$, $z_c = .440685....$ The singularities of various physical quantities are characterized by the corresponding critical exponents. The critical exponents of the Ising model are known. In particular, the bulk specific heat C diverges logarithmically at z_c, in standard notation, the corresponding critical exponents $\alpha = \alpha' = O_{\log}$ (see [22]).

Next, we will give the definitions of the thermodynamic quantities associated with the boundary. We consider an infinitely long ferromagnetic Ising strip consisting of m parallel layers with free boundary condition. We have [23]

$$\phi_m = \phi + 2m^{-1}f + o(m^{-1}). \tag{2.7}$$

where ϕ_m is the free energy per spin of the strip. ϕ ,as before, is the thermodynamic limit, f is the free energy per unit boundary length, $m^{-1}f$ stands for the correction due to the boundary

effect. In (2.7), the factor 2 befor $m^{-1}f$ comes from the two boundaries, upper and lower. (In some references, for example [23], this factor is omitted). It should be pointed out that for the infinitely long Ising strip each unit boundary length corresponds to one spin located on the boundary, thus more precisely, f is the free energy per unit boundary length and for this boundary every unit length corresponds to one statistical degree of freedom. From (2.7) the boundary free energy per unit length in the thermodynamic limit is defined as

$$f = 2^{-1} \lim_{m \to \infty} m (\phi_m - \phi). \tag{2.8}$$

Then, the boundary internal energy is

$$e = -\frac{\partial f}{\partial z}. \tag{2.9}$$

The boundary specific heat is

$$c^b = z^2 \frac{\partial e}{\partial z}. \tag{2.10}$$

It is clear that the equations similar to (2.8) which relate the boundary thermodynamic quantities with the corresponding bulk ones hold for e and c^b.

In the two-dimensional Ising model there is only one critical point, i.e. the singularities in the boundary thermodynamic quantities occur exactly at the same temperature as those in the bulk properties. It is known that in the thermodynamic limit e diverges logarithmically at z_c and superimposed on the logarithmic infinity, there is a discontinuity in e at z_c, i.e.

$$\lim_{\delta_z \to 0_+} (e (z_c + \delta_z) - e (z_c - \delta_z)) = L. \tag{2.11}$$

In the situation of free edges $L = 2^{-1}$ (if the factor 2 in (2.7) is omitted, L should be 1). In physics this phenomenon can be explained by "latent heat". The boundary specific heat c^b admits a singularity t^{-1} ($t = \frac{T}{T_c} - 1$), which means that c^b has opposite signs above and below T_c. The critical exponents of c^b are $\alpha_s = \alpha_s' = 1$. [22]

Now the problem is to evaluate the thermodynamic quantities for the Ising model and to obtain the critical information.

3. A Family of Methods Based on the Linkage Algorithm

In this section we introduce the linkage algorithm and the factored solution. Then we demonstrate that a family of methods can be derived by the linkage algorithm followed by factoring. It will be shown that the usual transfer matrix method is included in this family and the particular factored solution used in [10] is the best member in this family. In essence the factored operation is equivalent to an extrapolation. Thus this family of methods is characterized by successive increases in the lattice size followed by extrapolation.

In [10], the linkage algorithm and the factored solution have been described in detail. Here we only outline them. To compute the partition function of a lattice model we can consider that the lattice consists of some basic blocks. A basic block is an $m \times m$ array of spins; in the simplest case it can be a single spin. The partition function of the basic block is computed beforehand and subdivided into a sum parameterized by its leading spin configurations, e.g., the spin configuration which are located on the upper and right sides of the block. Then to construct the partition function of a large block, one can start with a small block, and repeatedly adjoin to it basic blocks on the left and bottom. The reader should refer to [10] for the computational formulas.

We consider an $N \times N$ two-dimensional Ising model and denote the partition function by $Z_{N \times N}$. In [10] Chorin has shown that the successive linkage of blocks results in an approximate factorization of the partition function into terms associated with small blocks far from the unconnected edge, and

$$\lim \frac{1}{N^2} \log Z_{N \times N} = \frac{1}{m^2} \log \tilde{Z}_{m \times m}, \tag{3.1}$$

where $\tilde{Z}_{m \times m}$ is the limiting factor. If we start with a block A, then by the linkage algorithm we can obtain

$$Z_B = \frac{Z_{A \bigcup B}}{Z_A}, \tag{3.2}$$

where Z_B is the contribution of the newly connected block B to the partition function of the lattice $A \bigcup B$. If Z_B obtained in successive linkage converge to a limit $\tilde{Z}$, then from (2.1) we obtain the approximation of the free energy $\phi_{N \times N} \rightarrow \phi$. In [10] it has been shown that the formulas for the free energy can be differentiated with respect to Z and yield successive approximations $U_{N \times N} \rightarrow U$, $C_{N \times N} \rightarrow C$.

In practice we perform computation only on a finite size lattice; thus it is impossible to obtain the limit of Z_B. The alternative approach is to compute Z_B only one time, i.e., if the whole lattice is denoted by $A \bigcup B$, we can start with a sub-lattice A, which is chosen properly, then the corresponding Z_B is used as $\tilde{Z}$ in (3.1).

The linkage algorithm is very flexible; the sub-lattice A can be chosen in many different ways. For example, for an $m \times n$ lattice some possible choices of A are shown in Fig.1. For each choice of A we can obtain a solution from (3.2) and (3.1). Thus in fact we have a family of methods. Each member of this family corresponds to a choice of A. In [10], a particular choice of A, as shown in Fig.1a, is used. The numerical tests have shown that, with this particular choice of A, the results are more accurate than with the others. This choice accelerates the convergence to the thermodynamic limit. For convenience, from now on, we call the method corresponding to the particular choice of A the particular factored solution, and the general operation expressed by (3.2) the factored operation.

Now we show that the usual transfer matrix method is a member of the family.

Consider an $m \times n$ Ising model. The partition function is given by (2.2). Denote a column configuration by σ_j, i.e.,

$$\sigma_j = (\mu_{1,j}, \mu_{2,j}, \ldots, \mu_{m,j}),$$

then there is a total of 2^m possible configurations for each σ. We can associate each configuration with an integer between 1 and 2^m according to the rule

$$\sigma = \sigma(i), \quad i \to 1 + \sum_{k=1}^{m} \max(0, \mu_k)\, 2^{k-1}.$$

If we define

$$V_1(\sigma_j) = -\sum_{i=1}^{m-1} \mu_{i,j}\, \mu_{i+1,j};$$

$$V_2(\sigma_j, \sigma_{j+1}) = -\sum_{i=1}^{m} \mu_{i,j}\, \mu_{i,j+1},$$

then, the partition function (2.2) can be written as

$$\begin{aligned} Z_{m \times n} &= -\sum_{\{\mu\}} \exp(-zE(\mu)) \\ &= \sum_{\sigma_1 \cdots \sigma_n} \exp(-z(\sum_{j=1}^{n} V_1(\sigma_j) + \sum_{j=1}^{n-1} V_2(\sigma_j, \sigma_{j+1}))) \\ &= \sum_{\sigma_1 \cdots \sigma_n} \exp(-\frac{z}{2} V_1(\sigma_1)) L(\sigma_1, \sigma_2) L(\sigma_2, \sigma_3) \cdots L(\sigma_{n-1}, \sigma_n) \exp(-\frac{z}{2} V_1(\sigma_n)), \end{aligned} \tag{3.3}$$

where

$$L(\sigma, \sigma') = \exp(-\frac{z}{2} V_1(\sigma)) \exp(-z V_2(\sigma, \sigma')) \exp(-\frac{z}{2} V_1(\sigma')) \tag{3.4}$$

is the (σ, σ') component of the 2^m by 2^m matrix L. The matrix L is called the transfer matrix. If we define a vector $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_{2^m})^T$, $\alpha_i = \exp(-\frac{z}{2} V_1(\sigma(i)))$, $i = 1, 2, \ldots, 2^m$, then (3.3) can be expressed as

$$Z_{m \times n} = (\alpha, L^{n-1} \alpha). \tag{3.5}$$

From (3.5) we know that, if we compute the partition function for an $m \times (n+1)$ lattice by linkage algorithm and construct the lattice by successive adjoing column to columns, it is equivalent to computing a series of expressions which have the same form as (3.5) and adjoing a column is equivalent to raising one power of L. If we consider the factored operation, as shown in Fig.1b, we take $Z_{A \cup B} = Z_{m \times (n+1)}$, $Z_A = Z_{m \times n}$, i.e., the lattice B is a column, we have

$$\begin{aligned} \phi_{m,n+1} &= \frac{1}{m}\log\frac{(\alpha, L^{n}\alpha)}{(\alpha, L^{n-1}\alpha)} \\ &= \frac{1}{m}(\log\lambda_1 + O((\frac{\lambda_2}{\lambda_1})^{n-1}))), \end{aligned} \tag{3.6}$$

where λ_1 is the largest eigenvalue of the 2^m by 2^m matrix L. For sufficiently large n, $\phi_{m,n}$ is a better approximation to $m^{-1}\log\lambda_1$ - the free energy per spin of an infinitely long Ising strip consisting of m layers. For fixed m, this approximation has an error $O((\frac{\lambda_2}{\lambda_1})^n)$. However, if we compute the free energy directly from (2.3) and use the result as an approximation to $m^{-1}\log\lambda_1$, the error is $O(n^{-1})$. Therefore, the method (3.6) allows an easy extrapolation from an $m \times n$ lattice to an $m \times\infty$ one, this is an advantade. In fact, from (3.6) we know that the factored operation carried out by taking B as a column is equivalent to computing the maximum eigenvalue of the transfer matrix L by the power method. It accelerates the convergence to the thermodynamic limit, but the accuracy obtained by this method is restricted by m. It is only an extrapolation along one direction i.e., the direction along which n increases. It is clear that the method (3.5), (3.6) is a member of the mentioned family. In essence it is the transfer matrix method but carried out in an implicit way. From now on, the method will be called the factored solution by column.

The factored solution by column has a lower accuracy than the particular factored solution. Visually, the reason is that, as shown in Fig.1a, the particular factored solution includes the extrapolation along two directions. Now we explain in detail why the particular factored solution accelerates the convergence to the thermodynamic limit and show that it is the best member of the mentioned family.

It is well known that phase transitions in statistical mechanical calculations arises only in the thermodynamic limit. The thermodynamic limit requires that the number of spins contained in a lattice system approach infinity. However, in any practical computation only finite lattices can be considered [4] [7]. An important part of the finite-size effect is due to the "dangling bonds" on the boundary [23]. In the two dimensional Ising model a general spin has four adjacent spins. A pair of adjacent spins are interrelated through a bond and interact with each other. However, the spins located on the boundary sites have no interaction with the outside, thus the contribution

of a boundary spin to the thermodynamic quantities differs from that of an inside spin. Since a unit boundary length corresponds to a dangling bond, this effect is proportional to the boundary length for the whole lattice system.

We inspect the particular factored solution from the point of view of boundary effects. It is found that although the rectangular lattice $A \bigcup B$ and the sub-lattice A in Fig.1a contain different number of spins, they have the same boundary length. As a consequence, they contain almost the same boundary effect induced by the "dangling bonds". Therefore, when the factored operation is executed, the effect is canceled. That is the reason why the particular factored solution may be a better approximation to the one in the thermodynamic limit.

From the above discussion it is plausible that the particular factored solution is better than the factored solution by column. For the factored solution by column, the lattice $A \bigcup B$ is an $m \times (n+1)$ rectangle and the sub-lattice A is an $m \times n$ one. They have different boundary length. After the factored operation some boundary effects induced by the "dangling bonds" are still included in the numerical results. Thus, the particular factored solution is more accurate.

To demonstrate that the particular factored solution is the best member of the family, we have need to show that the particular factored solution is more accurate than any methods in this family for which the lattice A has the same boundary length as the whole rectangular lattice. One example of such method is represented by Fig.1c.

We can only answer this question qualitatively and will be concerned with the spin effects which are located on corners. Until now the corner spin effect has not been clear, but the following discussion appears to be reasonable. The reader should refer to [4] [7] [23] for related discussions.

Let us first analyze the boundary effect induced by "dangling bonds" for an $m \times n$ lattice. For this lattice the boundary length is $2(m+n)$. There are $2(m+n)$–4 spins located on the boundary. The boundary length is not equal to the boundary spin number because there are four convex corners. Each spin located on a convex corner occupies two units of boundary. Thus the boundary spin number is four less than the boundary length. If the $2(m+n)$–4 spins were inside, they

would interact with $2(m+n)$ spins which were surrounding them outside. Thus we can consider that the boundary effect is equal to the interactions between the $2(m+n)$–4 boundary spins and the $2(m+n)$ imaged spins. Now we inspect the sub-lattice A shown in Fig.1a. It is found that it still has the boundary length $2(m+n)$. However, the boundary spin number reduces to $2(m+n)$–5, because there are five convex corners in the A. On the other hand, the spin number which are surrounding this sub-lattice A is $2(m+n)$–1. This number is one less than the number for an $m \times n$ lattice. The reason is similar, there is also a concave corner for the A. The two boundary spins which form the concave corner would only interact with one imaged spin outside A. Thus the boundary effects due to the "dangling bonds" for this A can be considered as the interaction between $2(m+n)$–5 boundary spins and $2(m+n)$–1 imaged spins. It is noticed that both the boundary spin number and the imaged spin number are one less than in an $m \times n$ lattice. Thus the boundary effects due to "dangling bonds" for the whole lattice and the sub-lattice A in Fig.1a are not exactly the same; they are only approximately equal to each other. Further, if we consider a general choice of sub-lattice A, it has still the boundary length $2(m+n)$, but l ($l \geq 5$) convex corners (in the example shown in Fig.1c, $l=7$). It is clear that any choice of this kind corresponds to a method of the family (the corresponding numerical result will be called the general factored solution). In company whth the l convex corners there must be l–4 concave corners. Thus for a general choice of A, the boundary effects can be considered as the interactions between $2(m+n)$–l boundary spins and $2(m+n)$–$(l-4)$ imaged spins. It is convinced that the bigger the number l is, the more different are the boundary effects between the $m \times n$ lattice and the sub-lattice A. Consequently, after the factored operation more boundary effects will remain in $\log Z_B$. It affects the accuracy strongly.

From the above discussion we know that the particular factored solution is the best member of this family, because in Fig.1a $l=5$, it is the possible minimum value. Thus, for the particular factored solution the boundary effects due to the "dangling bonds" are canceled almost thoroughly.

In addition, it should be noted that the boundary effects due to the "dangling bonds" for the particular factored solution are only eliminated approximately, thus if the difference between the whole lattice and the sub-lattice A is only a few spins located on the left and bottom corner, still the result is not satisfactory.

Table Ia
Convergence of factored solution by column to the free energy ϕ

z	$\phi_{4,5}$	$\phi_{8,9}$	$\phi_{12,13}$	$\phi_{8\times\infty}$	ϕ(exact)
.1	.7020	.7026	.7028	.7026	.7032
.2	.7291	.7318	.7327	.7318	.7345
.3	.7770	.7838	.7860	.7838	.7906
.4	.8496	.8645	.8694	.8645	.8794
.45	.8967	.9188	.9266	.9189	.9436
.5	.9515	.9843	.9968	.9845	1.026
.6	1.083	1.143	1.166	1.144	1.210
.7	1.237	1.321	1.349	1.321	1.404
.8	1.404	1.504	1.537	1.504	1.602
.9	1.576	1.689	1.720	1.689	1.801
1.0	1.750	1.876	1.917	1.876	2.001

Table Ib
Convergence of factored solution by column to the internal energy U

z	$U_{4,5}$	$U_{8,9}$	$U_{12,13}$	$U_{8\times\infty}$	U(exact)
.1	.1774	.1904	.1947	.1904	.2034
.2	.3699	.3991	.4088	.3991	.4282
.3	.5944	.6495	.6679	.6495	.7045
.4	.8664	.9826	1.023	.9831	1.106
.45	1.019	1.196	1.271	1.199	1.513
.5	1.174	1.421	1.533	1.419	1.746
.6	1.446	1.717	1.796	1.720	1.909
.7	1.620	1.812	1.862	1.810	1.964
.8	1.702	1.846	1.891	1.846	1.985
.9	1.734	1.861	1.905	1.861	1.993
1.0	1.745	1.868	1.911	1.868	1.997

Table Ic
Convergence of factored solution by column to the specific heat C

z	$C_{4,5}$	$C_{8,9}$	$C_{12,13}$	$C_{8\times\infty}$	C(exact)
.1	.0182	.0196	.0201	.0196	.0210
.2	.0822	.0899	.0925	.0899	.0977
.3	.2219	.2543	.2650	.2543	.2863
.4	.4742	.6312	.7021	.6353	.8626
.45	.6285	.9163	1.100	.9294	1.605
.5	.7627	1.066	1.140	1.002	.7249
.6	.8215	.5928	.4307	.5546	.3134
.7	.5951	.2535	.2213	.2584	.1581
.8	.3240	.1380	.1233	.1474	.0830
.9	.1480	.0808	.0698	.0877	.0441
1.0	.0604	.0477	.0399	.0444	.0234

Table IIa

Convergence of general factored solution ($l=7$) to the free energy ϕ

z	4×4 array	8×8 array	12×12 array	ϕ(exact)
.1	.7032	.7032	.7032	.7032
.2	.7345	.7345	.7345	.7345
.3	.7901	.7905	.7905	.7906
.4	.8754	.8785	.8790	.8794
.45	.9310	.9383	.9404	.9436
.5	.9960	1.011	1.016	1.026
.6	1.153	1.188	1.200	1.210
.7	1.337	1.387	1.398	1.404
.8	1.537	1.590	1.598	1.602
.9	1.744	1.792	1.798	1.801
1.0	1.953	1.995	1.999	2.001

Table IIb

Convergence of general factored solution ($l=7$) to the internal energy U

z	4×4 array	8×8 array	12×12 array	U(exact)
.1	.2034	.2034	.2034	.2034
.2	.4274	.4282	.4282	.4282
.3	.6943	.7032	.7042	.7045
.4	1.022	1.079	1.094	1.106
.45	1.205	1.320	1.369	1.513
.5	1.392	1.576	1.663	1.746
.6	1.724	1.923	1.945	1.909
.7	1.942	2.019	1.994	1.964
.8	2.047	2.031	2.004	1.985
.9	2.082	2.026	2.005	1.993
1.0	2.086	2.020	2.004	1.997

Table IIc

Convergence of general factored solution ($l=7$) to the specific heat C

z	4×4 array	8×8 array	12×12 array	C(exact)
.1	.0210	.0210	.0210	.0210
.2	.0967	.0976	.0976	.0977
.3	.2662	.2828	.2853	.2863
.4	.5714	.7166	.7806	.8626
.45	.7567	1.038	1.223	1.605
.5	.9201	1.221	1.303	.7249
.6	1.015	.6915	.3767	.3134
.7	.7617	.1674	.0941	.1581
.8	.3994	-.0053	.0214	.0830
.9	.1187	-.0543	-.0030	.0441
1.0	-.0049	-.0645	-.0106	.0234

Table IIIa
Convergence of particular factored solution to the free energy ϕ

z	4×4 array	8×8 array	12×12 array	ϕ(exact)
.1	.7032	.7032	.7032	.7032
.2	.7345	.7345	.7345	.7345
.3	.7904	.7905	.7906	.7906
.4	.8769	.8789	.8792	.8794
.45	.9339	.9396	.9411	.9436
.5	1.001	1.014	1.019	1.026
.6	1.163	1.196	1.205	1.210
.7	1.355	1.396	1.402	1.404
.8	1.560	1.579	1.601	1.602
.9	1.769	1.798	1.800	1.801
1.0	1.979	1.999	2.000	2.001

Table IIIb
Convergence of particular factored solution to the internal energy U

z	4×4 array	8×8 array	12×12 array	U(exact)
.1	.2034	.2034	.2034	.2034
.2	.4280	.4282	.4282	.4282
.3	.6997	.7041	.7044	.7045
.4	1.043	1.089	1.099	1.106
.45	1.239	1.345	1.389	1.513
.5	1.440	1.617	1.699	1.746
.6	1.792	1.957	1.949	1.909
.7	2.004	2.017	1.980	1.964
.8	2.085	2.014	1.992	1.985
.9	2.094	2.008	1.997	1.993
1.0	2.078	2.005	1.999	1.997

Table IIIc
Convergence of particular factored solution to the specific heat C

z	4×4 array	8×8 array	12×12 array	C(exact)
.1	.0210	.0210	.0210	.0210
.2	.0974	.0976	.0977	.0977
.3	.2743	.2851	.2860	.2863
.4	.6082	.7498	.8070	.8626
.45	.8139	1.108	1.302	1.605
.5	.9901	1.288	1.330	.7249
.6	1.043	.5614	.2388	.3134
.7	.6727	.0347	.0781	.1581
.8	.2236	-.0443	.0503	.0830
.9	-.0700	-.0352	.0282	.0441
1.0	-.2002	-.0231	.0134	.0234

4. A Extra Linear Extrapolation algorithm

In last section a family of methods has been discussed. Especially, in the family there are two specific members. One is the particular factored solution which is the best one of this family. The another is the factored solution by column which related to the usual transfer matrix method. In this section we discuss their further accelerations.

In [10] on the basis of the particular factored solution a further acceleration method which is called the scaling has been presented. The basic idea is as follows: We imagine a "spin bath" infinitely extending to the top and the right of a finite rectangular lattice. The spin bath imposes different weights on the configurations formed by the spins located on the top and the right boundary of the finite lattice. The method is an iterative one. It starts with a guess of the weights, then the particular factored solution is computed for the lattice with spin bath. From the computation a set of new weights are obtained by a method which can be considered as a reverse Kadanoff scaling. Thus the iterative process continues until convergence. In [10] some value of ϕ, U, C computed by the scaling method for 4×4 Ising model has been displayed. The convergence to the thermodynamic limit has not been proved.

In this paper we use the scaling method to compute the Ising model with different sizes. The results will be discussed in the next section. Here, we focus attention on the further acceleration of the factored solution by column.

From the last section we know that after the corresponding factored operation some boundary effects still remain in the factored solution by column. Now we inspect this point more precisely.

In Fig.1b, where the factored solution by column is sketched, $A \bigcup B$ is an $m \times (n+1)$ lattice and A is an $m \times n$ one. If we denote the free energy per spin computed with the linkage algorithm for lattice $A \bigcup B$ by $\phi_{m\times(n+1)}$, then the free energy of the whole lattice $A \bigcup B$ is $m(n+1)\phi_{m\times(n+1)}$. Similarly, for the lattice A the corresponding quantities is $mn\,\phi_{m\times n}$. When the factored operation is performed, the difference $m(n+1)\phi_{m\times(n+1)}-mn\,\phi_{m\times n}$ is computed. We study the difference in detail. Because $m(n+1)-mn=m$, in the difference there should be a term

which approximates to m-spin free energy. This term can be expressed approximately as $m\phi$, where ϕ, as before, is the free energy per spin in the thermodynamic limit. Moreover, some boundary effects are included in the difference. For the lattice $A \bigcup B$ and sub-lattice A shown in Fig.1b, the vertical boundaries have the same length, but in the horizontal direction the boundary of $A \bigcup B$ is one unit longer than the boundary of A. If we notice that there are two horizontal boundaries, up and down, and recall that the boundary effect per unit length is denoted by f in section 2, then there should be a term $2f$ in the difference. In Summary, if we denote the difference by $m\,\phi_{m,n+1}$, we have

$$\begin{aligned} m\,\phi_{m,n+1} &= m(n+1)\phi_{m\times(n+1)} - mn\,\phi_{m\times n} \\ &= \log\frac{Z_{m\times(n+1)}}{Z_{m\times n}} \\ &= m\phi + 2f + o(1), \end{aligned} \tag{4.1}$$

where $o(1)$ denotes the error due to the other finite-size effects and goes to zero as m, n tend to infinity. As compared with (3.6) it is clear that the $\phi_{m,n+1}$ defined by (4.1) is none other than the factored solution by column. And we know that the term $2f$ in (4.1) reduces the accuracy of $\phi_{m,n+1}$ as an approximation to ϕ. However, the term can be eliminated easily. Beside $\phi_{m,n+1}$ we compute $\phi_{m-1,n}$, according to (4.1),

$$(m-1)\phi_{m-1,n} = (m-1)\phi + 2f + o(1). \tag{4.2}$$

Subtracting (4.2) from (4.1), we have

$$\begin{aligned} \tilde{\phi}_{m,n+1} &= m\,\phi_{m,n+1} - (m-1)\phi_{m-1,n} \\ &= \phi + o(1) \end{aligned} \tag{4.3}$$

$\tilde{\phi}_{m,n+1}$ is a better approximation to ϕ than the factored solution by column $\phi_{m,n+1}$. Similar approximations to the bulk internal energy U and the bulk specific heat C can be derived in the same way and will be denoted by $\tilde{U}_{m,n+1}$ and $\tilde{C}_{m,n+1}$ respectively.

Here, it should be pointed out that to eliminate the term $2f$ from (4.1) we can use any $\phi_{p,q}$, the only requirement is $p \neq m$. We chose $\phi_{m-1,n}$ just for the convenience of programming.

In the practical computation we take $n = m$.

In the following the expression (4.3) is explained in a different way. If the $m \times n$ Ising model is wrapped on a torus and in the thermodynamic limit n is alowed to approach infinity before m, following Thompson [22], we have

$$\begin{aligned} \phi &= \lim_{m \to \infty} m^{-1} \log \lambda_1 = \frac{1}{2} \log (2\sinh (2z)) + \lim_{m \to \infty} (2m)^{-1} \sum_{k=0}^{k=m-1} \gamma_{2k+1} \\ &= \frac{1}{2} \log (2\sinh ((2z)) + (2\pi)^{-1} \int_0^{\pi} \cosh^{-1}(\cosh (2z) \coth (2z) - \cos(\theta))\, d\theta, \end{aligned} \tag{4.4}$$

where λ_1, as before, is the maximum eigenvalue of the 2^m by 2^m transfer matrix L and γ_k is defined by $\cosh(\gamma_k) = \cosh(2z)\coth(2z) - \cos(\frac{\pi k}{m})$. From (4.4) we know that using $m^{-1}\log\lambda_1$ instead of ϕ approximately corresponds to using the summation $(2m)^{-1} \sum_{k=0}^{k=m-1} \gamma_{2k+1}$ instead of the integral. From the point of view of numerical analysis this means that the integral is calculated by rectangle rule formula, and the number of intervals is proportional to m. On the other side from (3.6) we know that the factored solution by column $\phi_{m,n+1}$ is an approximation to $m^{-1}\log\lambda_1$. Thus we see that the algorithm expressed by (4.3) is none other than the Romberg method in numerical analysis, which improves the accuracy of the approximate integral calculation. From now on (4.3) will be called the extra linear extrapolation algorithm.

From (4.1) and (4.2) we can also derive a formula to compute the boundary free energy f. However, we should make a further assumption on the term $o(1)$ appearing in (4.1). Denotin the term by $\psi(m, n+1)$, we assume not only $\psi(m, n+1) \to 0$ as $m, n \to \infty$, but also

$$m\,\psi(m-1, n) - (m-1)\psi(m, n+1) \to 0, \quad as \quad m, n \to \infty. \tag{4.5}$$

This assumption means that either the term $o(1)$ has a higher order than m^{-1} or its main part can be expressed as $Am^{-\alpha}$, $0 < \alpha \leq 1$ and the coefficient A is independent of m. In fact, it seems reasonable to consider the term $o(1)$ very close to the difference between the free energy

computed for a finite lattice with periodic conditions and the corresponding thermodynamic limit. If it is true, then this term will decay exponentially with m. In the end of this section the validity of this assumption will be discussed by considering the high-temperature expansion for the boundary free energy f. Mainly it will be justified by the numerical results which are derived from this assumption and will be presented in the next section.

Under the assumption (4.5), multiplying (4.2) by m, and subtracting the result from $(m-1)\times(4.1)$, we have

$$f_{m,n+1} \equiv 2^{-1} m\,(m-1)(\phi_{m-1,n} - \phi_{m,n+1}) = f + o\,(1); \tag{4.6}$$

$f_{m,n+1}$ can be taken as an approximation to the boundary free energy per unit length.

It is clear that similar expressions hold for the approximation to the boundary internal energy and the approximation to the boundary specific heat. They are denoted by $e_{m,n+1}$, $c^{b}{}_{m,n+1}$, respectively.

From (4.6) an expression for the boundary free energy f of an infinitely long Ising strip can be derived. The expression (4.6) can be written as

$$\lim_{m,n\to\infty} 2^{-1} m\,(m-1)(\phi_{m-1,n} - \phi_{m,n+1}) = f. \tag{4.7}$$

In (4.7) we allow n go to infinity before m, then

$$\lim_{m\to\infty} 2^{-1} m\,(m-1)(\phi_{m-1} - \phi_{m}) = f\ , \tag{4.8}$$

where

$$\phi_m = \lim_{n\to\infty} \phi_{m,n+1} = \frac{1}{m} \log \lambda_1, \tag{4.9}$$

it can be obtained from (3.6) and λ_1 is the maximum eigenvalue of the 2^m by 2^m matrix L given

by (3.4). Here for indicating the dependence of λ_1 on m, we denote it by $\lambda_1(m)$. Thus the expression (4.8) can be written as

$$f = \lim_{m\to\infty} \frac{1}{2} \log \left(\frac{{\lambda_1}^m (m-1)}{{\lambda_1}^{m-1}(m)}\right). \tag{4.10}$$

Expression (4.10) exhibits the relation between the eigenvalues of the transfer matrix and the boundary thermodynamic functions.

Now we briefly discuss the validity of the assumption (4.5). In order to show that the assumption (4.5) is reasonable, we will compare the f defined by (2.8) with the expression (4.7) which is derived on the basis of (4.5). However, it is difficult to do this analytically, instead, we adopt an alternative way, i.e., we compare the two high-temperature expansions for f which are derived from (2.8) and (4.7) separately, and consider only the first few terms.

It is well known that in high temperature the free energy ϕ can be expanded as a series in $\omega = tanh(z)$ and the expansion coefficients can be calculated by a combinatorial approach (see [22]). If we only consider the first few terms of the series, the corresponding coefficients can be obtained easily and ϕ can be written as

$$\phi = \log 2 + 2\log\, cosh(z) + \omega^4 + 2\omega^6 + \frac{9}{2}\omega^8 + O(\omega^{10}). \tag{4.11}$$

For the free energy of an $m \times n$ Ising model with free edges, the corresponding expansion is

$$\phi_{m\times n} = \log 2 + (2-(\frac{1}{m}+\frac{1}{n}))\log\, cosh(z) + (\frac{1}{m}-1)(\frac{1}{n}-1)\omega^4 + (2-3(\frac{1}{m}+\frac{1}{n})+\frac{4}{mn})\omega^6$$
$$+(\frac{9}{2}-\frac{21}{2}(\frac{1}{m}+\frac{1}{n})+\frac{43}{2}\frac{1}{mn})\omega^8 + O(\omega^{10}). \tag{4.12}$$

In (4.12) let n go to infinity, we have

$$\phi_m = \log 2 + (2-\frac{1}{m})\log\, cosh(z) + (1-\frac{1}{m})\omega^4 + (2-\frac{3}{m})\omega^6 + (\frac{9}{2}-\frac{21}{2m})\omega^8 + O(\omega^{10}). \tag{4.13}$$

Substituting (4.11) and (4.13) into (2.8), or substituting (4.12) into (4.7), we obtain the same expansion:

$$f = -2^{-1}(\log \cosh z + \omega^4 + 3\omega^6 + \frac{21}{2}\omega^8) + O(\omega^{10}). \tag{4.14}$$

To some extent this result shows us that the assumption (4.5) is reasonable. Here we have only considered the coefficients of the terms to ω^9 because when the power increases the computation of the corresponding coefficient becomes very complicated.

Table IVa
Convergence of scaling method to the free energy ϕ

z	4×4 array	8×8 array	12×12 array	ϕ(exact)
.1	.7032	.7032	.7032	.7032
.2	.7345	.7345	.7345	.7345
.3	.7908	.7906	.7906	.7906
.4	.8808	.8795	.8794	.8794
.45	.9433	.9424	.9426	.9436
.5	1.019	1.021	1.023	1.026
.6	1.197	1.205	1.208	1.210
.7	1.392	1.400	1.402	1.404
.8	1.593	1.599	1.601	1.602
.9	1.794	1.799	1.800	1.801
1.0	1.996	1.999	2.000	2.001

Table IVb
Convergence of scaling method to the internal energy U

z	4×4 array	8×8 array	12×12 array	U(exact)
.1	.2034	.2034	.2034	.2034
.2	.4285	.4282	.4282	.4282
.3	.7098	.7045	.7044	.7045
.4	1.121	1.110	1.107	1.106
.45	1.381	1.418	1.441	1.513
.5	1.621	1.700	1.731	1.746
.6	1.900	1.923	1.919	1.909
.7	1.990	1.979	1.971	1.964
.8	2.013	1.995	1.990	1.985
.9	2.016	2.000	1.997	1.993
1.0	2.014	2.002	1.999	1.997

Table IVc
Convergence of scaling method to the specific heat C

z	4×4 array	8×8 array	12×12 array	C(exact)
.1	.0210	.0210	.0210	.0210
.2	.0981	.0976	.0977	.0977
.3	.2970	.2865	.2860	.2863
.4	.7974	.8612	.8692	.8620
.45	1.057	1.327	1.504	1.605
.5	1.056	1.074	.9560	.7249
.6	.5642	.3539	.3096	.3134
.7	.2153	.1378	.1435	.1581
.8	.0572	.0572	.0703	.0830
.9	-.0090	.0212	.0255	.0441
1.0	-.0335	.0450	.0149	.0234

Table Va

Convergence of linear extrapolation algorithm to the free energy ϕ

z	$\tilde{\phi}_{4,5}$	$\tilde{\phi}_{8,9}$	$\tilde{\phi}_{12,13}$	ϕ(exact)
.1	.7032	.7032	.7032	.7032
.2	.7345	.7345	.7345	.7345
.3	.7906	.7906	.7906	.7906
.4	.8791	.8793	.8794	.8794
.45	.9389	.9416	.9423	.9436
.5	1.010	1.020	1.024	1.026
.6	1.187	1.209	1.210	1.210
.7	1.391	1.405	1.404	1.404
.8	1.602	1.602	1.602	1.602
.9	1.809	1.801	1.801	1.801
1.0	2.012	2.000	2.000	2.001

Table Vb

Convergence of linear extrapolation algorithm to the internal energy U

z	$\tilde{U}_{4,5}$	$\tilde{U}_{8,9}$	$\tilde{U}_{12,13}$	U(exact)
.1	.2034	.2034	.2034	.2034
.2	.4284	.4282	.4282	.4282
.3	.7062	.7045	.7045	.7045
.4	1.083	1.103	1.106	1.106
.45	1.312	1.398	1.432	1.513
.5	1.551	1.717	1.774	1.746
.6	1.943	1.967	1.912	1.909
.7	2.106	1.964	1.962	1.964
.8	2.099	1.980	1.985	1.985
.9	2.045	1.997	1.993	1.993
1.0	2.005	1.996	1.997	1.997

Table Vc

Convergence of linear extrapolation algorithm to the specific heat C

z	$\tilde{C}_{4,5}$	$\tilde{C}_{8,9}$	$\tilde{C}_{12,13}$	C(exact)
.1	.0210	.0210	.0210	.0210
.2	.0979	.0977	.0977	.0977
.3	.2874	.2864	.2863	.2863
.4	.6970	.8213	.8524	.8620
.45	.9644	1.321	1.548	1.605
.5	1.173	1.413	1.171	.7249
.6	1.026	.0580	.1981	.3134
.7	.2680	.0418	.1722	.1581
.8	-.2966	.0996	.0866	.0830
.9	-.4129	.0636	.0445	.0441
1.0	-.2950	.0323	.0234	.0234

Table VIa
The maximum specific heats $C^{max}_{m,m}$ and their positions $z^c_{m,m}$ computed by the particular factored solution

m	4	6	8	10	12
$z^c_{m,m}$	.56114	.51726	.49690	.48511	.47742
$C^{max}_{m,m}$	1.0800	1.1944	1.2892	1.3695	1.4389

Table VIb
The maximum specific heats $C^{max}_{m,m}$ and their positions $z^c_{m,m}$ computed by the scaling method

m	4	6	8	10
$z^c_{m,m}$	.47440	.46478	.459921	.45566
$C^{max}_{m,m}$	1.0954	1.2359	1.3448	1.4336

Table VIc
The maximum specific heats $C^{max}_{m,m+1}$ and their positions $z^c_{m,m+1}$ computed by linear extrapolation algorithm

m	4	6	8	10	12
$z^c_{m,m+1}$	.53413	.49737	.48148	.47258	.46687
$C^{max}_{m,m+1}$	1.2227	1.3686	1.4846	1.5784	1.6579

* See section 5 for the meaning of the symbols $C^{max}_{m,n}$ and $z^c_{m,n}$.

* In the thermodynamic limit the bulk specific heat diverges logarithmically at $z_c = .440685.....$

Table VIIa

The boundary free energy f computed by the linear extrapolation algorithm

z	$f_{4,5}$	$f_{8,9}$	$f_{12,13}$
.1	-.0025	-.0025	-.0025
.2	-.0108	-.0108	-.0108
.3	-.0273	-.0271	-.0271
.4	-.0590	-.0595	-.0596
.45	-.0843	-.0911	-.0945
.5	-.1179	-.1413	-.1576
.6	-.2071	-.2610	-.2680
.8	-.3962	-.3935	-.3911
1.0	-.5231	-.4977	-.4974
1.5	-.7577	-.7548	-.7499
2.0	-1.001	-.9999	-1.000
2.5	-1.250	-1.250	-1.250

Table VIIb

The boundary internal energy e computed by linear extrapolation algorithm

z	$e_{4,5}$	$e_{8,9}$	$e_{12,13}$
.1	.0519	.0519	.0519
.2	.1170	.1166	.1166
.3	.2236	.2199	.2198
.4	.4324	.4824	.4937
.45	.5865	.8066	.9678
.5	.7546	1.184	1.447
.6	.9938	1.001	.7511
.8	.7932	.5332	.5556
1.0	.5192	.5127	.5158
1.5	.4739	.5007	.5007
2.0	.4952	.5000	.5000
2.5	.4993	.5000	.5000

Table VIIc

The boundary specific heat c^b computed by linear extapolation algorithm

z	$c^b_{4,5}$	$c^b_{8,9}$	$c^b_{12,13}$
.1	.0056	.0056	.0056
.2	.0315	.0309	.0309
.3	.1310	.1283	.1279
.4	.4457	.7605	.9013
.45	.6718	1.620	2.682
.5	.8206	1.388	.1822
.6	.4094	-2.139	-1.395
.8	-1.241	-.1535	-.2206
1.0	-.7111	-.0615	-.0988
1.5	-.1658	-.0010	-.0101
2.0	-.0710	-.0009	-.0009
2.5	-.0171	-.0001	-.0001

Table VIII

The boundary free energy f computed by formula (4.10)

z	$m=4$	$m=5$	$m=6$	$m=7$	$m=8$	$m=9$
.1	-.0025	-.0025	-.0025	-.0025	-.0025	-.0025
.2	-.0108	-.0108	-.0108	-.0108	-.0108	-.0108
.3	-.0271	-.0271	-.0271	-.0271	-.0271	-.0271
.4	-.0573	-.0583	-.0588	-.0591	-.0593	-.0594
.45	-.0812	-.0846	-.0870	-.0888	-.0901	-.0913
.5	-.1129	-.1213	-.1276	-.1329	-.1367	-.1402
.6	-.1954	-.2130	-.2303	-.2480	-.2588	-.2634
.7	-.2777	-.3117	-.3277	-.3318	-.3326	-.3328
.8	-.3667	-.3873	-.3906	-.3910	-.3910	-.3910
.9	-.4377	-.4447	-.4452	-.4452	-.4452	-.4452
1.0	-.4954	-.4973	-.4974	-.4974	-.4974	-.4974

5. Some Numerical Result

In this section we present some numerical results. First, the approximate bulk thermodynamic functions computed by the different factored solutions as well as by the two further accelaration methods, i.e., the scaling and the extra linear extrapolation algorithm, are given. From these results the different methods can be compared. Furthermore, the boundary thermodynamic functions computed by the extra linear extrapolation algorithm are displayed, from which the algorithm is tested.

For the bulk thermodynamic functions, our results can be compared with [17], in which the $N \times N$ Ising model with free edges has been computed by the Monte-Carlo method for $N \leq 100$. All of our methods, i.e., the particular factored solution, the scaling and the extra linear extrapolation, have shown much faster convergence than the corresponding Monte-Carlo. If we inspect the maximum bulk specific heat values and their positions, this point will be shown more clearly. For example, the maximum specific heat computed by the extra linear extrapolation algorithm for a 10×11 lattice is 1.5784 which occurs at $z = .47258$, however, if we want to obtain a comparable result by Monte-Carlo, at least the lattice size needs to exceed 40×40. For the boundary thermodynamic functions of the Ising model our numerical result are apparently the first and their convergence looks good. The approximate boundary free energy, internal energy and specific heat are consistent with the theoretical predictions and reveal the specific features of the thermodynamic limit functions. From the finite lattice data the critical exponents can be recognized. The comparision for the critical point estimates will be discussed in the next section. Our estimate is also better than the Monte-Carlo's and comparable with the numerical renormalization group results in e.g., [18] [20].

In Tables 1a, 1b, 1c we disply $\phi_{m,m+1}$, $U_{m,m+1}$, $C_{m,m+1}$ computed by factored solution by column for m =4,8,12 and some z. For the sake of comparison the corresponding valus for a $8\times\infty$ lattice as well as the exact values of ϕ, U, C are also given. In Tables 2a, 2b, 2c and 3a, 3b, 3c we disply $\phi_{m\times m}$, $U_{m\times m}$, $C_{m\times m}$ computed by the general (l=7) and the particular fac-

tored solution for the same m and z, respectively. We see that the results computed by the factored solution by column for finite lattices are almost the same as those for an infinitely long Ising strip, i.e., this method accelerates the convergence to the thermodynamic limit. However, because of the boundary effects due to "dangling bonds" even though the lattice size for the factored solution by column, which is $m \times (m+1)$, is larger than the corresponding lattice size for the general or particular factored solution, which are $m \times m$, in Table 1 the finite lattice quantities converge to the thermodynamic limit slower than in Table 2 or 3. This result means that the accuracy of the factored solution by column is the lowest among the three methods. The reason has been explained in section 3. When we compare Table 2 with Table 3 we find that the results in Table 3 are more accurate. These results indicate that the particular factored solution used in [10] is the best member in the family of approximate factorization methods.

In Tables 4a, 4b, 4c and 5a, 5b, 5c displayed are the same thermodynamic functions computed by the scaling method and the extra linear extrapolation algorithm. For the scaling method the lattices are $m \times m$. For the extra linear extrapolation algorithm, according to formula (4.3) and similar ones, the relevant maximum lattice size is $m \times (m+1)$. However the computational labor required by the scaling is still much more than the latter because it is an iterative algorithm and use spin bath.

From Tables 4 and 5, we find that the solutions of the scaling method and the extra linear extrapolation algorithm are more accurate than the particular factored solutions. For small size of lattice, for example $m = 4$, the scaling method appears to be more accurate than the extrapolation algorithm. However, if we consider the whole results, these two algorithms have comparable accuracy. It is also found that for fixed z, when the lattice size increases, for both the scaling and the extra linear extrapolation algorithm the results converge to the thermodynamic limit. In Fig.2 the variation of the approximate bulk specific heat $\tilde{C}_{m \times (m+1)}$ computed by the extra linear extrapolation algorithm with z is shown. Under the condition of finite-size lattice, the logarithmic singularity in the specific heat transforms into a smooth peak. When the lattice size increases, the peak moves to the critical point, at the same time the width of the peak becomes narrow and the

height of the peak increases. It suggests that the critical exponents be $\alpha=\alpha' =0$. It is also noticed that the curve of the approximate specific heat given by the extra linear extrapolation algorithm for fixed m has a small oscillation at $z > z_c$. When m increases the amplitude of the oscillation is reduced and the position at which the oscillation occurs moves to the critical point. If we carefully observe the particular factored solution similar phenomenon can be found. However, for the factored solution the oscillation is mild. Without separating the boundary effect this phenomenon could not be observed.

In tables 6a, 6b and 6c, the maximum bulk specific heat values $C^{\max}{}_{m,n}$ computed for some $m \times n$ lattices and the temperatures $z^c{}_{m,n}$ at which the corresponding maximum occurs are shown. These data are computed by the particular factored solution, the scaling method and the extra linear extrapolation algorithm. For the scaling method the data are restricted to $m \leq 10$, because the amount of the computational labour for $m =12$ is too large for this method and our computer VAX 780. However, for the particular factored solution and the extra linear extrapolation algorithm a lattice with $m = 16$ can be computed on the same computer without difficulties. Table 6 shows that for the same (or nearly same) lattice size the maximum bulk specific heat obtained from the particular factored solution is less than those obtained from the scaling and the extra linear extrapolation algorithm. And the position at which the maximum occurs for the particular factored solution is farther from the critical point. If we compare the scaling with the extra linear extrapolation algorithm the situation is interesting. For the same m, the extrapolation algorithm gives a higher maximum specific heat, but the position of the maximum specific heat obtained by the scaling is more close to the critical point.

In Tables 7a, 7b and 7c the approximate boundary free energy $f_{m,m+1}$, the approximate boundary internal energy $e_{m,m+1}$, the approximate boundary specific heat $c^b{}_{m,m+1}$ computed by formula (4.6) and similar ones are tabulated for $m =4, 8, 12$. The curves of $f_{m,m+1}$, $e_{m,m+1}$ and $c^b{}_{m,m+1}$ vs. z for $m =5, 10, 15$ are shown in Fig. 3a, 3b and 3c, respectively. We have also computed the approximate boundary free energy by formula (4.10), where the principal eigenvalue of the transfer matrix L is computed directly by power method in double precision. This compu-

tation requires more storage space and CPU time, thus we can only compute (4.10) for small m. For m =4, 5, 6, 7, 8, 9 the results are displayed in Table 8.

From Table 7a and Table 8, it is found that the boundary free energy computed by the extra linear extrapolation algorithm is very close to those computed by formula (4.10). it seems that for the same m (4.10) gives more accurate result because it considers an infinitely long Ising strip. We also compute the boundary free energy by the series expansion (4.14) for z =.1,.2,.3,.4. The corresponding numerical results are −.0025, −.0108, −.0270, −.0562, respectively. They are very close to the results shown in Table 7a and 8, which signifies that the assumption (4.5) is reasonable and the formulas (4.6), (4.10), (4.14) that express the approximate or exact boundary free energy are correct.

Another interesting point is that from Table 7a, we guess that when the temperature goes to zero, the boundary free energy can be approximate by $-2^{-1}z$ very well.

In Fig.3b for the boundary internal energy as with the bulk specific heat, the logarithmic singularity is replaced by a smooth peak. As lattice size increases, the width of the peak becomes narrow and its position moves to the critical point from the low temperature side. In section 2 it has been stated that in the thermodynamic limit, superimposed on the logarithmic infinity, a discontinuity exists in e at z_c. Under the finite lattice condition this phenomenon is shown in the nonsymmetry of the $e_{m,m+1}$ curves. The interesting point is that although we have only calculated relatively small lattices, at the two ends of these $e_{m,m+1}$ curves the computed values appear to converge already. If we compare the values at the two ends, for example at z =.1 and z =2.5, it is found that for each m the difference is almost exact 0.5, i.e. the jump which happens at z_c in the thermodynamic limit.

In Fig. 3c for every m the two ends of the $c^b{}_{m,m+1}$ curve approach to the x-axis respectively from the positive and the negative direction. In the middle of the curve a positive maximum continuously but rapidly transforms into a negative minimum. This graph corresponds to the singularity t^{-1} in the thermodynamic limit. As m increases both the maximum and the minimum move to the critical point from the low temperature side, at the same time the distance

between them dicreases, however, the amplitude increases. It is predictable that the position of either the maximum or the minimum will coincide with z_c in the thermodynamic limit and the amplitude will go to infinity at the same time.

6. Discussion

In this section, we estimate the critical point by combining the different numerical results obtained by the particular factored solution, the scaling and the extra linear extrapolation algorithm with finite size scaling theory. Finaliy, we give a brief review of these methods.

In finite size scaling theory it is well known that the thermodynamic quantities of a lattice with linear dimension m are functions of m^{-1}, and the exact values in the thermodynamic limit, corresponding to $m^{-1}=0$ (i.e. m equals to infinity), can be extrapolated from the finite lattice results. For the numerical results obtained by the particular factored solution or the scaling method it is clear that they correspond to a linear dimension m, because they are all computed for $m \times m$ lattices. However, for the extra linear extrapolation algorithm both the bulk and the boundary free energy are linear combinations of two factored solutions by column, i.e. linear combinations of $\phi_{m,m+1}$ and $\phi_{m-1,m}$. We ask what is the linear dimension of these combinations. Recall that in section 3, we have demonstrated that the factored solution by column $\phi_{m,n}$ can be considered as an approximation to the free energy of an infinitely long strip consisting of m layers. Thus $\phi_{m,m+1}$ has a linear dimension m, similarly $\phi_{m-1,m}$ has a linear dimension $m-1$. Therefore, the numerical results obtained by the extra linear extrapolation algorithm should be considered as a function of $\tilde{m}^{-1}=2^{-1}(m^{-1}+(m-1)^{-1})$, i.e. the corresponding linear dimension is $\tilde{m}$. For convenience we use subscript m to denote quantities obtained by the extra linear extrapolation algorithm, but as soon as we are concerned with finite size scaling theory, $\tilde{m}$ should be used instead of m.

From the numerical computation we know that the approximate bulk specific heat obtained by any mentioned method for each finite lattice has an maximum which occurs at a certain temperature. Thus for every method this temperature can be considered as an m-dependent pseudo-

critical point. In Table 6, we displayed these maximum specific heat values and the corresponding pseudo-points obtained by the particular factored solution, the scaling and the extra linear extrapolation algorithm. Similarly, for the boundary thermodynamic functions we can also define the pseudo-critical point. For the boundary internal energy the pseudo-point is the temperature at which for a certain finite lattice the approximate boundary internal energy achieves its maximum value. For the approximate boundary specific heat, two different pseudo-critical points can be defined - one is the temperature at which the boundary specific heat achieves its maximum; the other is that at which the minimum boundary specific heat occurs. In Table 9 the pseudo-critical points and the corresponding maximum or minimum for the boundary thermodynamic functions are displayed. These data are computed by the extra linear extrapolation algorithm.

Table IX. The maximum or minimum of boundary thermodynamic functions and the pseudo-critical point computed by the extra linear extrapolation algorithm.

m	internal energy		max. specific heat		min. specific heat	
	e_{max}	$z^e{}_{max}$	$c^b{}_{max}$	$z^{cb}{}_{max}$	$c^b{}_{min}$	$z^{cb}{}_{min}$
4	1.0160	.63947	.82839	.51260	-1.2643	.82594
5	1.0941	.59313	1.0602	.49448	-1.4908	.72714
6	1.1627	.56515	1.3009	.48384	-1.7135	.66977
7	1.2235	.54623	1.5484	.47681	-1.9327	.63197
8	1.2777	.53250	1.8011	.47179	-2.1483	.60507
9	1.3264	.52205	2.0579	.46803	-2.3608	.58490
10	1.3704	.51380	2.3179	.46509	-2.5704	.56919
11	1.4105	.50711	2.5805	.46273	-2.7776	.55659
12	1.4471	.50158	2.8452	.46080	-2.9825	.54626
13	1.4809	.49691	3.1118	.45918	-3.1856	.53763
14	1.5121	.49293	3.3800	.45780	-3.3871	.53031
15	1.5411	.48948	3.6495	.45662	-3.5871	.52403

The real critical temperature can be estimated as follows. In Table 6 and Table 9, for every group of data which is given by one method for a certain thermodynamic function, the positions of the maxima or minima, i.e., the pseudo-critical points, vary with the lattice linear dimensions. It is found that there are very good linear relations between the pseudo-critical points and the reciprocal linear dimensions $\tilde{m}^{-1}$. Thus, if we assume that for each group of data, the pseudo-critical point is a linear function of $\tilde{m}^{-1}$, i.e., $z_{max\,(min)}=a_0+a_1\tilde{m}^{-1}$, then a_0 and a_1 can be estimated by least square method from the numerical results shown in Table 6 or Table 9 for every group of data. It is clear that the value of a_0 can be considered an estimate of the real critical point and this estimate depends not only on the type of pseudo-critical point but also on the lattice sizes which are concerned with in the least square computation.

In Table 10a the approximate critical points estimated from the maximum bulk specific heat are given. The data in different rows correspond to different methods which have been used to compute the bulk specific heat. In Table 10b the approximate critical points estimated from different boundary thermodynamic quantities are displayed.

Table Xa
The critical point estimated from maximum bulk specific heat values.

numerical method	lattice size	approximate critical point	lattice size	approximate critical point	lattice size	approximate critical point
factored solution	m =4, 6, 8, 10	.4346	m =6, 8, 10	.4373	m =8, 10	.4380
scaling method	m =4, 6, 8, 10	.4435	m =6, 8, 10	.4420	m =8, 10	.4415
extra linear extrapolation	m =4, 6, 8, 10	.4377	m =6, 8, 10	.4391	m =8, 10	.4395

Table Xb
The critical point estimated from boundary thermodynamic function computed by extra linear extrapolation algorithm

type of pseudo-critical point	lattice size	approximate critical point	lattice size	approximate critical point	lattice size	approximate critical point
maximum internal energy	m =11,12, 13,14,15	.4434	m =13,14, 15	.4432	m =14,15	.4430
maximum specific heat	m =11,12, 13,14,15	.4406	m =13,14, 15.	.4407	m =14,15	.4407
minimum specific heat	m =11,12, 13,14,15	.4388	m =13,14, 15	.4393	m =14,15	.4395

We recall that the exact critical point value is .440685.... From Table 10a, we know that the scaling method gives the best estimate for the critical point and for the particular factored solution the estimate has the lowest accuracy. For the scaling method if we use the pseudo-critical points with the linear dimension m =8, 10 in the least square computation the approximate critical point is .4415. The relative error is less than .002. However, it should be pointed out that the scaling method requires more computational labour than the other methods, it restrains us from computation of more large lattice on our computer. Thus we cannot obtain more exact estimate from the scaling. For the extra linear extrapolation algorithm if we use the pseudo-critical points for m =14, 15, we obtained the approximate critical point .4403, whose relative error is less than .001.

In Table 10b the estimates of the critical point obtained from the boundary thermodynamic functions are shown. From it we know that the estimate computed from the maximum boundary specific heat has the highest accuracy. In the least square method if we consider m =13, 14, 15, it gives the exact result in four significant digits. In the last column of Table 10b the maximum relative error is even only .005.

The above results can be compared with those obtained by other numerical methods. In [20], the approximate critical point computed by the cumulant expansion method has been given. The value is .4302 and has the relative error .011. In [17], the $N \times N$ Ising model for $N \leq 100$ have been computed by the Monte-Carlo method, and the author declared that the estimate for the critical point is correct to better than .005. It can be compared with the maximum error in the last column of Table 10b. In [18], Nightingale obtained some critical point estimates which are slightly better than ours, but it should be pointed out that in [18] , to estimate the critical point the analytic expression of the inverse correlation length of an $n \times \infty$ Ising strip has been used, thus it is not a "purely" numerical result.

Finally, we briefly review the particular factored solution, the scaling method and the extra linear extrapolation algorithm to end this paper.

The particular factored solution eliminates the finite-size effect due to the "dangling bonds" almost thoroughly. It is the best member in the factorization method family and accelerates the convergence of finite lattice quantities to the thermodynamic limit. Although its accuracy is lower than the scaling and the extra linear extrapolation algorithm, the method is very simple and can be easily combined with other methods, for example the Monte-Carlo method. Thus it is a desirable method.

The scaling method gives high accuracy, especially, when the lattice size is small. With the lattice size increasing, the thermodynamic functions computed by the scaling converge to their thermodynamic limits. From results the critical point can be estimated better. However, this method requires more computational time and storage space, this restricts its use. If we can combine this method with Monte-Carlo, it will produce a more efficient and flexible method. Idea somewhat similar to this approach has been considered by Goodman and Sokal [13].

The extra linear extrapolation algorithm also gives a high accuracy and does not need much increase of the computational labour. In addition, this algorithm can be used to compute the boundary thermodynamic functions and give satisfactory results. In further work we shall study how the boundary magnetic quantities for a lattice model can be computed with similar algorithms and try to combine the extra linear extrapolation algorithm with other methods.

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Fig.1. The skatch map of some possible choices of lattie A and B.

Fig.2. The bulk specific heat computed with the extra linear extrapolation algorithm. The triangles are the particular factored solution for m=12.

Fig.3a. The boundary free energy computed with the extra linear extrapolation algorithm.

Fig.3b. The boundary internal energy computed with the extra linear extrapolation algorithm.

Fig.3c. The boundary specific heat computed with the extra linear extrapolation algorithm.

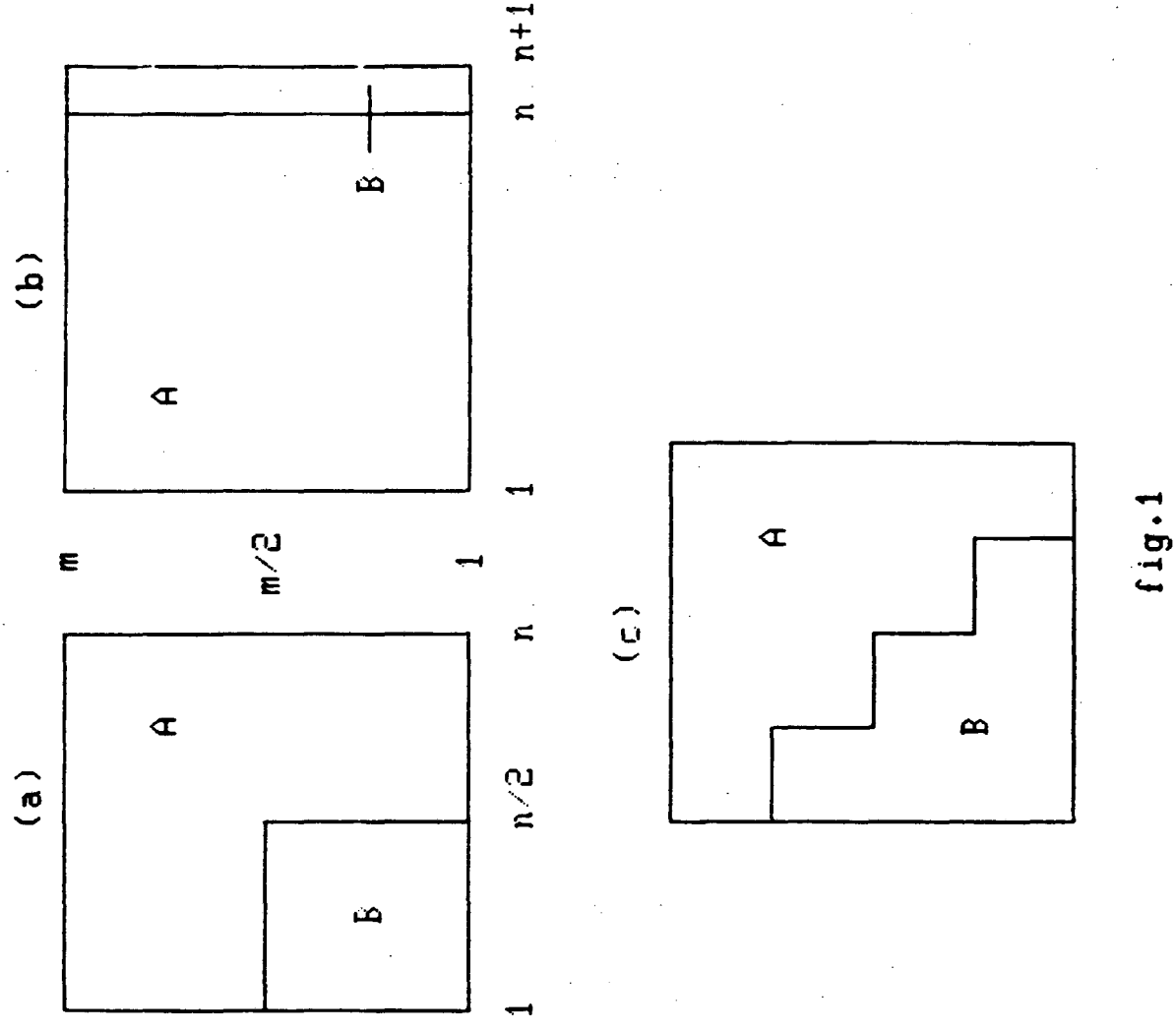
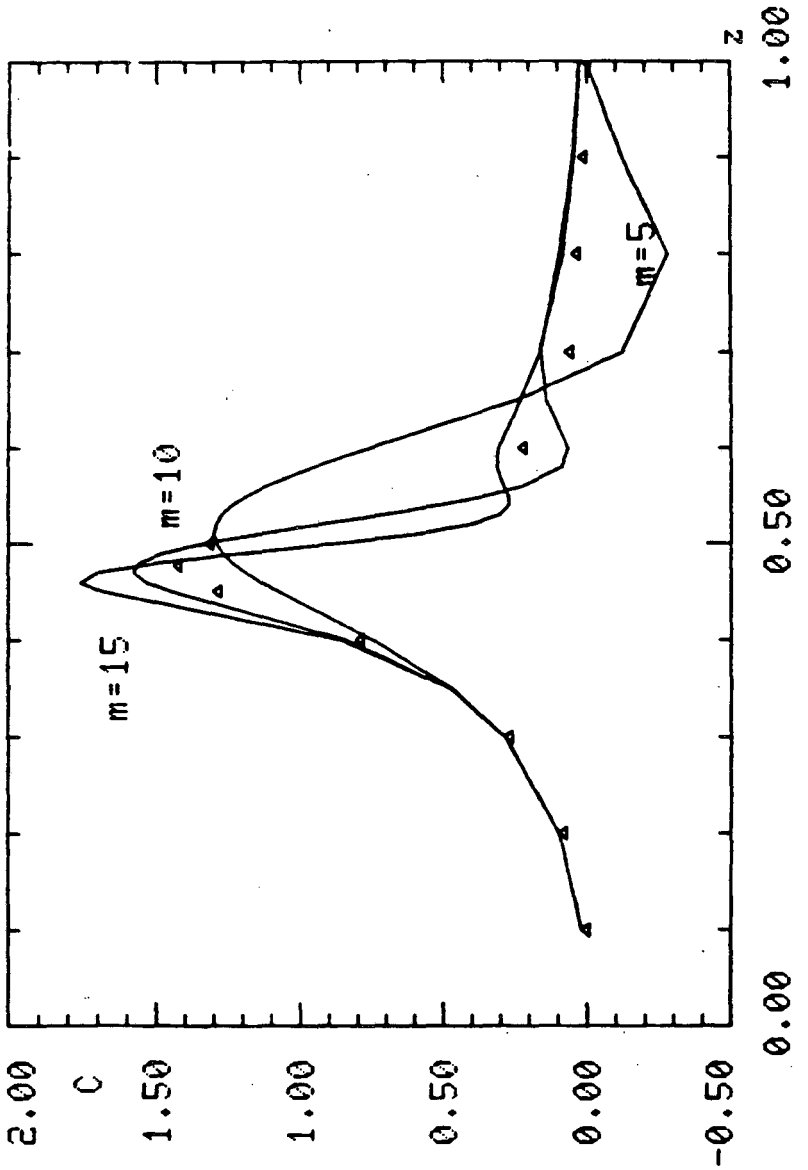


fig.1



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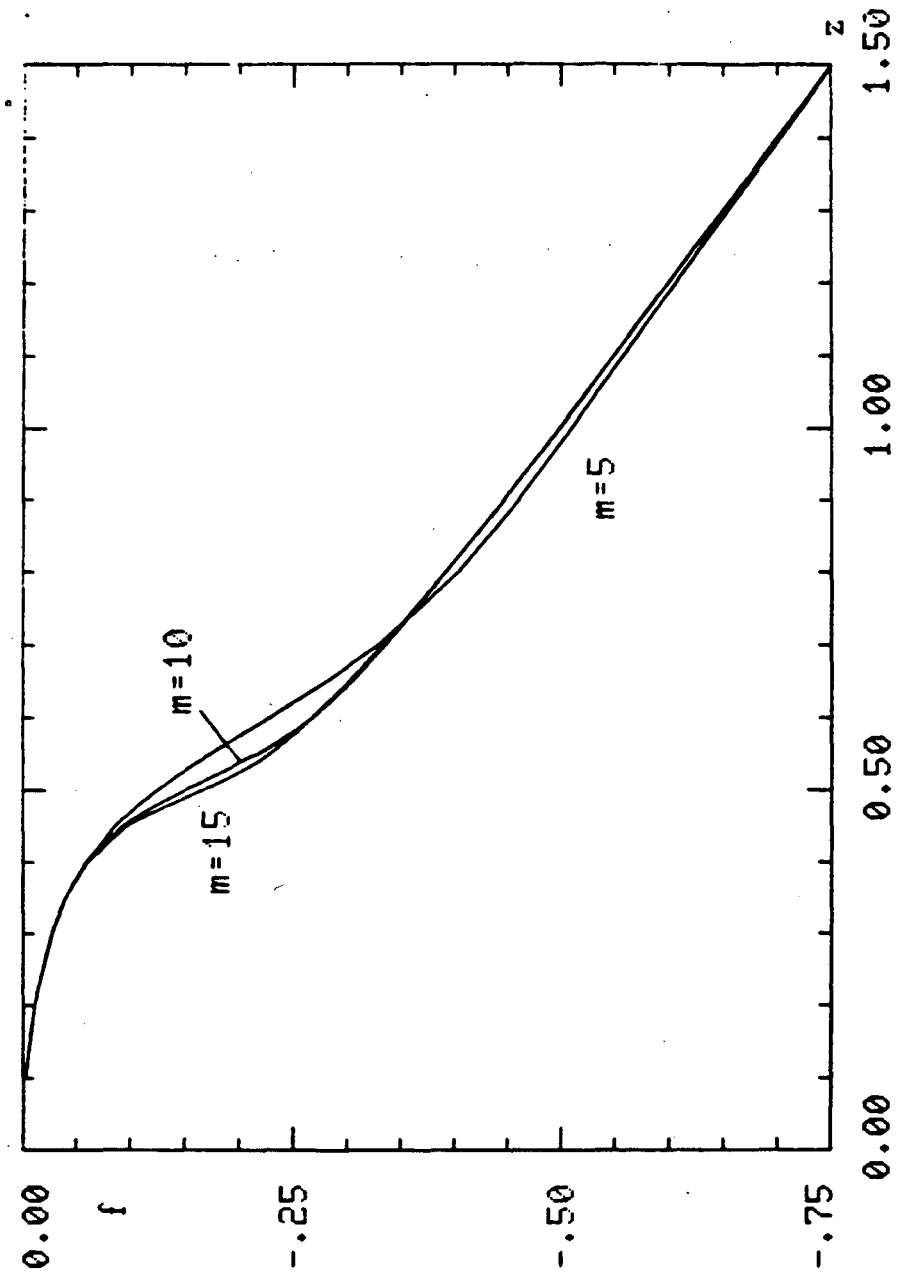

fig.3a

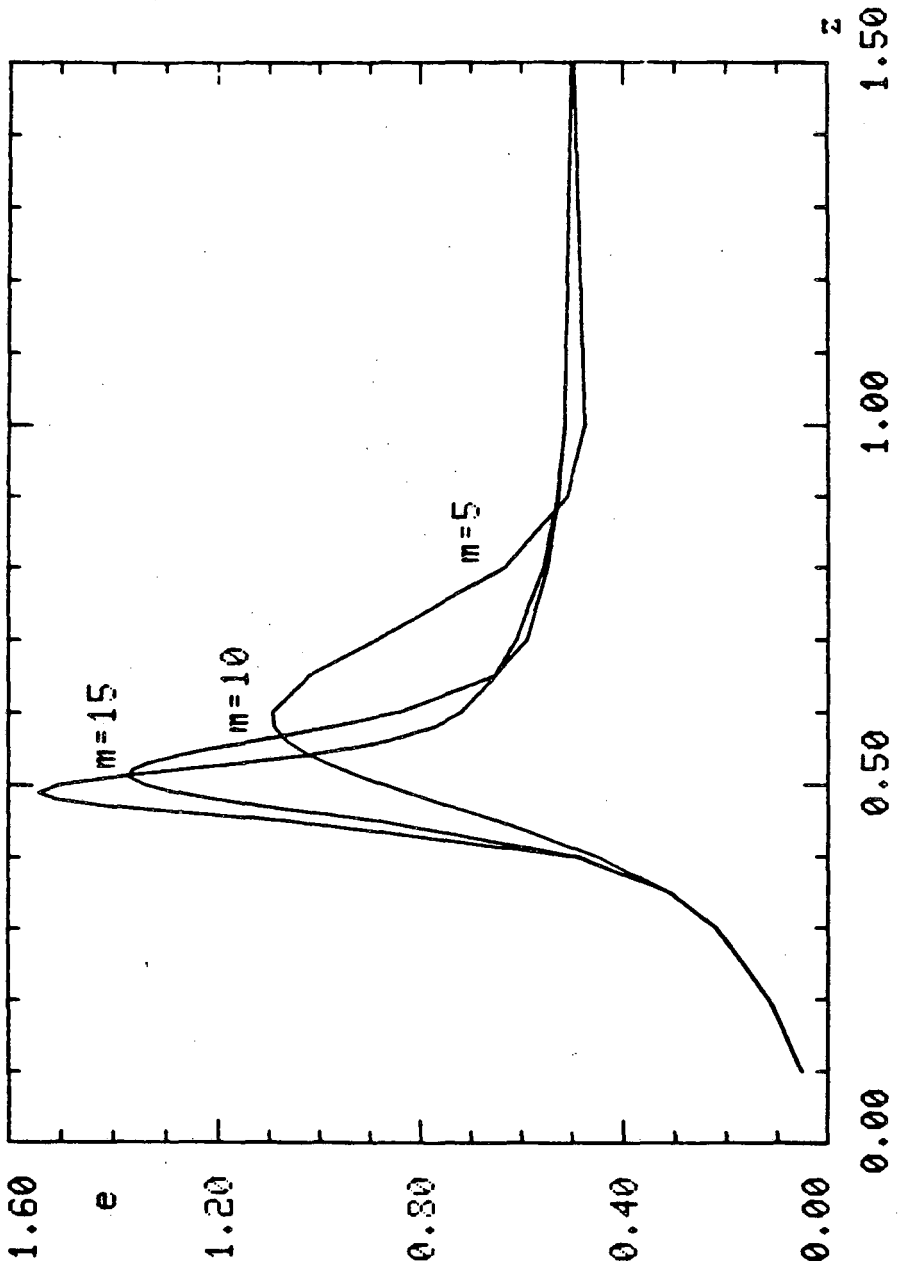

fig.3b

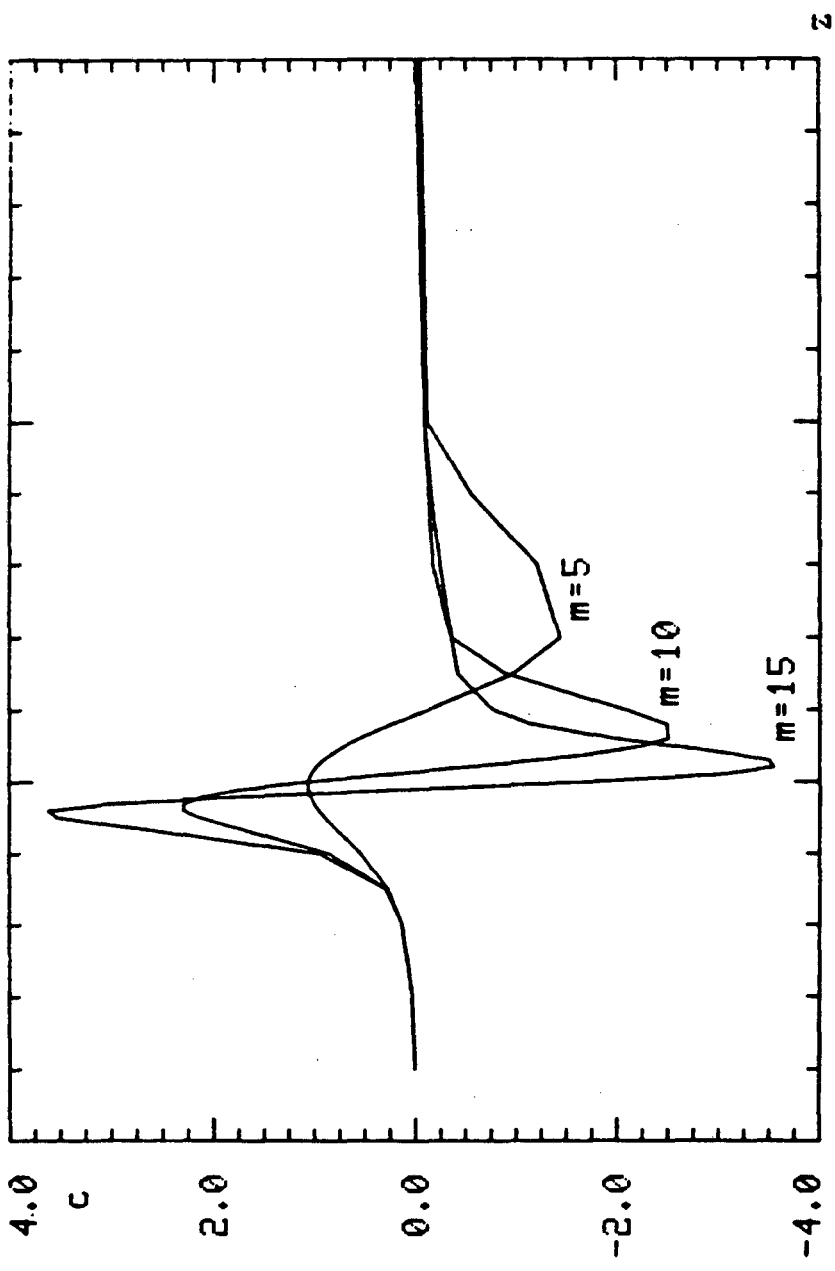

fig.3c

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