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October 1984

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SOLUTION OF LATTICE MODELS BY SUCCESSIVE LINKAGE[1]

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Abstract

A linkage algorithm is presented for evaluating the partition function of a union of finite lattice blocs in terms of the partition functions of the component blocs. This algorithm leads to: (i) A fast enumeration method for evaluating the partition function of a finite lattice (for Ising spins in two dimensions, the amount of labor in evaluating the partition function for a bloc of L spins is reduced from $O(2^L)$ to $2^{O(\sqrt{L})}$); (ii) a recursive factorization procedure that accelerates the rate at which quantities evaluated on a finite lattice converge to their thermodynamic limit, and (iii) a scaling procedure that further accelerates the convergence to the thermodynamic limit. The scaling procedure is similar to a method previously used in turbulence calculations.

Introduction

The goal of this paper is to present several methods for reducing drastically the amount of labor required to evaluate the partition function, the free energy and other thermodynamic quantities for a class of lattice models that includes the Ising model. The main tool is a linkage algorithm that relates the partition function and the free energy of a union of blocs to the same quantities evaluated on the component blocs. This linkage algorithm leads to an exact fast enumeration scheme that reduces drastically the labor required to evaluate the partition function of a finite lattice (for L Ising spins on the line, the amount of labor is reduced from $O(2^L)$ to $O(L)$; for L Ising spins in the plane, the reduction is from $O(2^L)$ to $2^{O(\sqrt{L})}$, and in three dimensions, from $O(2^L)$ to $2^{O(L^{2/3})}$). This fast enumeration procedure has features in common both with spatial renormalization [2] and with the fast Fourier transform. The linkage algorithm also leads to an approximate factorization of the partition function that allows quantities computed on a finite lattice to converge rapidly to their thermodynamic limit

(for Ising spins on the line, the thermodynamic limit is reached, after factorization, on a bloc of 4 spins). Finally, a scaling method, coupled to the linkage, further accelerates the convergence to the thermodynamic limit. The scaling resembles a mesh refinement in numerical analysis as well as a reverse Kadanoff scaling [5]. All these methods can be used in conjunction with the usual renormalization and Monte-Carlo methods [1], but our interest in them lies in the fact that they can be generalized to non-homogeneous systems and to fluid mechanics. In fact, the scaling algorithm is analogous to a method already used in a turbulence calculation [3],[4]. In the present paper, we explain the methods and apply them to the two-dimensional Ising model, where an exact solution affords a useful check.

To establish the notations, we briefly describe the ferromagnetic Ising model (see e.g. [9]). Consider an $N\times N$ square lattice with nodes (i,j), $1\le i\le N$, $1\le j\le N$, carrying spin $\mu_{i,j}$, $\mu_{i,j}=\pm 1$. A set of values $\mu=\{\mu_{i,j}\}$ is a configuration. The energy of a configuration, in appropriate units, is

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

The partition function is

$$Z_{N\times N} = \sum_{\mu} e^{-zE(\mu)},$$

where $z = 1/T$ and T is the temperature. The free energy $\varphi_{N\times N}$ for the finite lattice is

$$\varphi_{N\times N} = \frac{1}{N^2}\log Z_{N\times N}, \tag{2}$$

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

$$\varphi = \lim_{N\to\infty}\varphi_{N\times N}. \tag{3}$$

The internal energy U is

$$U = -\frac{\partial \varphi}{\partial z}, \tag{4}$$

and the specific heat C is

$$C = z^2 \frac{\partial U}{\partial z}. \tag{5}$$

We shall also find use for the quantities $U_{N\times N} = -\frac{\partial \varphi_{N\times N}}{\partial z}$, $C_{N\times N} = z^2 \frac{\partial U_{N\times N}}{\partial z}$. The Ising model admits a critical point z_c, i.e., a non-analytic point of φ; $\sinh 2z_c = 1$, $z_c = .440685\cdots$. The critical exponents are known; in particular, C diverges logarithmically at z_c ($\alpha = \alpha' = 0_{\log}$ in standard notation, see e.g. [8],[9]).

We shall also discuss the one-dimensional Ising model; its definition is obvious.

Linkage and factorization in one dimension. We begin by explaining the ideas in the trivial one-dimensional case. Consider a bloc of m spins, which we shall call the basic bloc. For simplicity, and without loss of generality, we shall write all the formulas in the simple case $m = 2$. The basic bloc has 4 configurations, $(+,+),(+,-),(-,+),(-,-)$, where $(+,-)$ refers to a configuration in which the left spin is +1 and the right spin is -1, etc. The partition function $Z^0 = Z_2$ of the basic bloc is

$$Z^0 = \Lambda_+^0 + \Lambda_-^0, \tag{6}$$

where $\Lambda_+^0 = e^z + e^{-z}$ is the contribution to the partition function of those configurations in which the left spin is +1, and $\Lambda_-^0 = e^z + e^{-z}$ is the contribution to Z^0 of those configurations in which the left spin is -1. (For pedagogical reasons, we resolutely refrain from noticing at this stage that $\Lambda_+^0 = \Lambda_-^0$.) We say that the partition function has been subdivided in (6) into terms parametrized by the leading spin on the left, or, for short, that it has been parametrized by the lead-

ing spin on the left, and we call the quantities $\Lambda_{\pm}^{O}$ the weights attached to the leading spin configuration.

Adjoin to the first bloc on the left another basic bloc with a partition function parametrized by the leading spin on the right; it is obvious that the parametrization by the left spin is identical to the parametrization by the right spin. The partition function Z_4 of the union of the two blocs is

$$Z_4 = \Lambda_{4,+} + \Lambda_{4,-}, \tag{7}$$

where

$$\Lambda_{4,+} = \Lambda_{+}^{O} e^{z} \Lambda_{+}^{O} + \Lambda_{+} e^{-z} \Lambda_{-}^{O}, \tag{8}$$

$$\Lambda_{4,-} = \Lambda_{-}^{O} e^{z} \Lambda_{-}^{O} + \Lambda_{-} e^{-z} \Lambda_{+}^{O}; \tag{9}$$

The middle factors $e^{\pm z}$ come from the interaction of the leading spins, and (7) is a parametrization by the second spin from the left. It is easy to see that in the one-dimensional case a parametrization by any one spin is identical to the parametrization by any other, and thus (7) is also the parametrization of Z_4 by the leading spin on the left. To obtain Z_6, one can adjoin to the bloc of 4 spins another basic bloc and find

$$Z_6 = \Lambda_{6,+} + \Lambda_{6,-},$$

where

$$\Lambda_{6,+} = \Lambda_{+}^{O} e^{z} \Lambda_{4,+} + \Lambda_{+}^{O} e^{-z} \Lambda_{4,-},$$

$$\Lambda_{6,-} = \Lambda_{-}^{O} e^{z} \Lambda_{4,-} + \Lambda_{-}^{O} e^{-z} \Lambda_{4,+};$$

etc. The amount of labor required to evaluate Z_N is obviously merely proportional to N; this is the linkage algorithm in this special case.

Write

$$Z_N = Z^{(1)} Z^{(2)} Z^{(3)} \ldots Z^{(l)}, \quad Z^{(1)} = Z^{O}, \tag{10}$$

with $ml = 2l = N$, where $Z^{(i)}$ is the factor by which $Z_{(i-1)l}$ is multiplied when

the i-th basic bloc is added. $Z^{(i)}$ can be viewed as the contribution of the i-th bloc to the total Z_N. Suppose $Z^{(i)} \to \tilde{Z}$, $\tilde{Z}$ independent of i. Then

$$\begin{aligned} \varphi = \lim_{N\to\infty} \frac{1}{N} \log Z_N &= \lim_{l\to\infty} \frac{1}{lm} \sum_{i=1}^{l} \log Z^{(i)} \\ &= \frac{1}{m} \log \tilde{Z}; \end{aligned} \tag{11}$$

thus, $\tilde{Z}$ determines φ and its derivatives. Equation (10) will be referred to as an approximate factorization of Z_N; formula (11), if $\tilde{Z}$ exists, is a better approximation to φ than can be obtained directly from a finite Z_N because the successive approximations to $\tilde{Z}$ afforded by the successive $Z^{(i)}$ rapidly forget the unconnected side of the starting bloc.

From (7),(8),(9) we find

$$Z^{(2)} = Z_4 / Z^{(1)} = \Lambda_+^{(2)} + \Lambda_-^{(2)} \tag{12}$$

where

$$\Lambda_+^{(2)} = \Lambda_+^0 \left(e^z \frac{\Lambda_+^0}{Z^{(1)}} + e^{-z} \frac{\Lambda_-^0}{Z^{(1)}} \right), \tag{13}$$

$$\Lambda_-^{(2)} = \Lambda_-^0 \left(e^z \frac{\Lambda_-^0}{Z^{(1)}} + e^{-z} \frac{\Lambda_+^0}{Z^{(1)}} \right), \tag{14}$$

i.e., $\Lambda^{(2)}$ consists of the terms in $Z^{(1)}$, modified by $e^{\pm z}$ and multiplied by the weights $\Lambda_\pm^0 / Z^{(1)}$ that can be viewed as the appropriate probabilities. Similarly,

$$Z^{(3)} = Z_6 / Z^{(2)} = \Lambda_+^{(3)} + \Lambda_-^{(3)}$$

where the $\Lambda_\pm^{(3)}$ consists of $\Lambda_\pm^0$, multiplied by the $e^{\pm z}$ and by appropriate probabilities obtained from $Z^{(2)}$.

Do the $Z^{(i)}$ converge? In the present one dimensional case we notice that, by symmetry, $\Lambda_+^{(i)} = \Lambda_-^{(i)}$ for all i, $\Lambda_+^{(i)} / Z^{(i)} = \frac{1}{2}$ for all $i > 1$, and thus for $i > 1$

$$\mathcal{Z}^{(i)} = (e^z + e^{-z})\left[e^z\ \frac{1}{2} + e^{-z}\ \frac{1}{2}\right] + (e^z + e^{-z})\left[e^z\ \frac{1}{2} + e^{-z}\ \frac{1}{2}\right],$$
$$= 4\cosh^2 z\ ;$$

thus $\mathcal{Z}^{(i)} = \mathcal{Z}$ for $i > 1$, and by (11)

$$\varphi = \frac{1}{2}\log(4\cosh^2 z) = \log(2\cosh z),$$

which is the well-known exact solution. The thermodynamic limit has been obtained, after factorization, in a system of 4 spins. If one uses one-spin blocs, the limit is reached in a system of 3 spins.

Successive linkage in two dimensions. In this section we generalize the constructions of the preceding section to the Ising model in two dimensions. We begin by introducing some notations. Let $s = (s^{(1)}, s^{(2)}, \ldots, s^{(m)})$ be an array of spins, i.e., variables taking on the values ± 1. To this array one can associate an integer between 1 and 2^m by the rule

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

Conversely, given an integer between 1 and 2^m and the dimension m of the array one can uniquely reconstruct the corresponding array. We shall assign the same labels to the arrays and the corresponding integers.

Given the two arrays s_1, s_2, one can construct the array which consists of the two laid side by side; we shall call both the new enlarged array and the corresponding integer $s_1 \oplus s_2$. Finally, given two arrays s_1, s_2 of the same length m, one can construct their inner product

$$(s_1, s_2)_m = (s_1, s_2) = \sum_{i=1}^{m} s_1^{(i)} s_2^{(i)}.$$

Consider an $m \times m$ array of spins (fig. 1), which we shall call a basic bloc. There are 2^{m^2} spin configurations. Suppose they are generated in some order and

tagged by an integer i, $1 \le i \le 2^{m^2}$. To each i there corresponds an energy $E(i)$, an m-array $s_S = s_S(i)$ of spins on the bottom of the square, and m-array $s_W = s_W(i)$ of spins on the left of the square, and similarly for s_E, s_N. (S stands for "south", W for "west", etc.) Furthermore, one can write

$$s_{SW} = s_S \oplus s_W \quad , \quad s_{NE} = s_N \oplus s_E \quad , \quad etc.$$

s_{SW} has $2m$ entries, and if the entries of s_S are enumerated from left to right and the entries of s_W are enumerated from top to bottom, then the first and $(m+1)$st entries of s_{SW} are equal, since the corner spin is common to s_S and s_W. The partition function for the basic bloc is

$$Z_B^Q = \sum_i e^{-zE(i)},$$

where $E(i)$ is given by (1) with $N = m$.

Suppose one is given the partition function for a bloc A of spins, and suppose one picks out a finite array of sites on the edge of A, and suppose one knows how to write

$$Z_A = \sum_s \Lambda_s^A \tag{15}$$

where the sum is over all configurations in the edge array. We shall again say that Z_A has been subdivided into a sum parametrized by the leading spin configurations, and we shall call the Λ_s^A the corresponding weights. Thus, if s has two entries, one expects

$$Z_A = \Lambda_{(+,+)}^A + \Lambda_{(+,-)}^A + \Lambda_{(-,-)}^A + \Lambda_{(-,+)}^A.$$

Suppose the leading edge of the given bloc A is such that one can attach to it a basic bloc without gaps or overlaps, (fig. (2)). Suppose the leading spin array is written as

$$s = s_1 \oplus s_l \oplus s_2,$$

where s_i contains all the spin sites abutting on the added bloc, and s_1, s_2 are the disjoint, possibly empty, arrays on either side. The partition function for the union of the old bloc A and the basic bloc B is

$$Z_{A\cup B} = \sum_{s_1,s_2} \sum_{j=1}^{2^{2m}} \sum_{i=1}^{2^{m^2}} \Lambda^A_{s_1\oplus j\oplus s_2} e^{z(j,s_{NE}(i))_e - zE(i)}. \tag{16}$$

The two outer sums in equation (16) are over all relevant boundary configurations, the remaining sum is over all configurations in the bloc being linked, and the exponential in the middle represents the interactions between the old bloc and the new bloc. Furthermore, $Z_{A\cup B}$ can be parametrized by the new leading configurations $s_1 \oplus k \oplus s_2$ by adding a term

$$\Lambda_{s_1\oplus j\oplus s_2} e^{z(j,s_{NE}(i))_e - zE(i)} \tag{17}$$

to $\Lambda^{A\cup B}_{s_1\oplus k\oplus s_2}$ whenever $k = s_{SW}(i)$. To construct the partition function of a large bloc, one can start with a small bloc, and repeatedly adjoin to it blocs on the left and bottom, or in any two neighboring directions. If one views the cost of summing over i as a fixed overhead, then the cost of finding the partition function for an $N\times N$ bloc is, except for negligible factors, determined by the length of the moving edge of the computed bloc, i.e., it is of order $2^{O(N)}$, where $N = \sqrt{L}$, L = total number of spins.

A particularly simple case is one in which one constructs Z for the union of only four blocs (fig. 3). The formulas for this special case will be given in the next section.

As in the one-dimensional case, the successive linkage of blocs results in an approximate factorization of the partition function into terms associated with small blocs far from the unconnected edge, and

$$\lim_{N\to\infty} \frac{1}{N^2} \log Z_{N\times N} = \frac{1}{m^2} \log \tilde{Z}_{m\times m} \tag{18}$$

where $\tilde{Z}_{m\times m}$ is the limiting factor.

Indeed, if one writes

$$Z_B = Z_{A\cup B} / Z_A ,$$

where Z_B is the contribution of the newly connected basic bloc to the partition function, one finds

$$Z_B = \sum_{s_1,s_2} \sum_i e^{-zE(i)} \sum_j e^{z(j,s_{NE}(i))} (\Lambda^A_{s_1\oplus j\oplus s_2} / Z_A), \tag{19}$$

with $\sum(\Lambda^A_{s_1\oplus j\oplus s_2} / Z_A) = 1$ by (15). Once again, the intra-bloc partition function is modified by exponential interaction terms multiplied by suitable probabilities. If the Z_B obtained in successive linkages converge to a limit $\tilde{Z}$, equation (18) holds. Note that equations (16),(18) can be differentiated with respect to z and yield successive approximations $U_{N\times N} \to U$, $C_{N\times N} \to C$. Note further that (16),(19) remain valid and are particularly simple when Z_B consists of a single spin.

Some numerical results. In this section, we present some numerical results obtained with the fast enumeration and approximate factorization algorithms. On a computer, some simple precautions must be taken to avoid problems with round-off errors and with overflow. First, all exponentials of the form e^{zl}, l integer, should be stored in the form $e^{(zl-\alpha z)}$, with α chosen in each part of the calculation so that $l-\alpha \leq 0$ for all the relevant l. Z is then modified by a multiplicative factor, $\log Z$ by an additive factor, U and C are unchanged; the modifications are readily taken into account. Furthermore, the Λ's can become quite large and must be scaled into a reasonable range. If the approximate factorization is used, the scaling of Λ^A_s does not change Z_B. We assume from now on that these precautions have been taken.

We shall use in this section the four bloc union of fig. 3. The formulas then become particularly simple. The general formula (16) will be used in the next section.

Suppose Z_B^Q, the partition function of the basic bloc, has been parametrized by $s_S \oplus s_\nu$,

$$Z_B^Q = \sum_{s_S \oplus s_\nu} \Lambda_{s_S \oplus s_\nu}.$$

The partition function of the two bloc configuration, (fig. 3), parametrized by $s_S \oplus s_2$, is

$$Z^{2\ blocs} = \sum_{s_S \oplus s_2} \Lambda^{2\ blocs}_{s_S \oplus s_2},$$

where

$$\Lambda^{2\ blocs}_{s_S \oplus s_2} = \sum_{s_\nu} \sum_{s_1} \Lambda^{O}_{s_S \oplus s_\nu} e^{z(s_\nu, s_1)} \Lambda^{O}_{s_1 \oplus s_2}.$$

In the next step

$$Z^{3\ blocs} = \sum_{s_S \oplus s_4} \Lambda^{3\ blocs}_{s_S \oplus s_4},$$

where

$$\Lambda^{3\ blocs}_{s_S \oplus s_4} = \sum_{s_2} \sum_{s_3} \Lambda^{2\ blocs}_{s_S \oplus s_2} e^{z(s_2, s_3)} \Lambda^{O}_{s_3 \oplus s_4},$$

and finally $Z_{2m \times 2m}$ is

$$Z_{2m \times 2m} = Z^{4\ blocs} = \sum_{s_5 \oplus s_6} \sum_{s_S \oplus s_4} \Lambda^{3\ blocs}_{s_S \oplus s_4} e^{z(s_S \oplus s_4, s_5 \oplus s_6)} \Lambda^{O}_{s_S \oplus s_4}. \qquad (20)$$

The last and best $m \times m$ factor in the approximate factorization is

$$Z_{m \times m} \cong Z^{4\ blocs} / \sum', \qquad (21)$$

where

$$\sum' = \sum_{s_5 \oplus s_4} \Lambda^{3\ blocs}_{s_5 \oplus s_4}.$$

For example, the cost of computing $Z_{4\times4}$ is $O(2^{16})$; the cost of computing $Z_{8\times8}$ by the algorithm just described is $\sim 4 \cdot O(2^{16})$; the cost of evaluating $Z_{8\times8}$ directly, without linkage, is $O(2^{64})$. Our algorithm reduces the amount of labor by a factor of $\sim 2^{64}/(4 \cdot 2^{16}) \cong 2^{44} \cong 10^{11}$. Furthermore, by the factorization we approach the thermodynamic limit closer than an 8×8 bloc would otherwise allow. Our evaluation of $Z_{8\times8}$ takes about 3 minutes on a VAX 780 small computer.

In tables Ia, Ib, Ic we display $\varphi_{m\times m}$, $U_{m\times m}$, $C_{m\times m}$, computed by formula (20), for $m = 4,6,8$ as well as the exact values of φ, U, C for some value of z. We see that the finite lattice quantities converge very slowly to the thermodynamic limit. In tables IIa, IIb, IIc, we display the factored approximation (21) for $2m = 4,6,8$; in all cases, the factored approximation approaches the limit much faster than the corresponding unmodified arrays. For $z > z_c$ the convergence is in fact quite good; above but not far from the critical point the convergence is still rather poor for the derivatives of φ; for a discussion of the reasons and a partial remedy, see the next section. The variation of the factored approximation with z is displayed in figs. 4, 5, and 6. The approximations to φ and U on the finite lattice look quite good, but of course the correct critical behavior is not reached on this small finite lattice, as one can observe from the approximation of C in fig. 6. Still, if one knew there was a singularity in C, one could locate it between $z = .41$ and $z = .51$ -- not a bad result for an 8×8 lattice. Furthermore, the characteristic exponent α is clearly 0, assuming a singularity exists. These results are not substantially poorer than the numerical renormalization group results in e.g. [6],[7].

Table Ia

Convergence of $\varphi_{N\times N}$ to the free energy φ

z	$\varphi_{4\times4}$	$\varphi_{6\times6}$	$\varphi_{8\times8}$	φ (exact solution)
.2	.7238	.7274	.7291	.7345
.4	.8241	.8416	.8507	.8794
.45	.8623	.8863	.8991	.9434
.5	.9061	.9385	.9563	1.026
.7	1.132	1.209	1.253	1.404
1.	1.551	1.690	1.764	2.000

Table Ib

Convergence of $U_{N\times N}$ to the internal energy U

z	$U_{4\times4}$	$U_{6\times6}$	$U_{8\times8}$	U (exact)
.2	.3140	.3515	.3705	.4282
.4	.7067	.8212	.8845	1.106
.45	.8194	.9681	1.056	1.513
.5	.9324	1.118	1.233	1.746
.7	1.287	1.520	1.637	1.964
1.	1.461	1.645	1.734	1.997

Table Ic

Convergence of $C_{N\times N}$ to the specific heat C

z	$C_{4\times4}$	$C_{6\times6}$	$C_{8\times8}$	C (exact)
.2	.0681	.0778	.0826	.0686
.4	.3549	.4540	.5200	.8557
.45	.4604	.6096	.7200	1.607
.5	.5573	.7362	.8596	.7155
.7	.5827	.4981	.4074	.1302
1.	.2123	.1274	.0941	.0198

Table IIa

Convergence of factored approximations to the free energy φ

z	4×4 array	6×6 array	8×8 array	φ (exact)
.2	.7345	.7345	.7345	.7345
.4	.8769	.8784	.8789	.8794
.45	.9340	.9379	.9396	.9434
.5	1.001	1.009	1.014	1.026
.7	1.355	1.384	1.395	1.404
1.	1.978	1.996	1.999	2.000

Table IIb

Convergence of factored approximations to the internal energy U

z	4×4 array	6×6 array	8×8 array	U (exact)
.2	.4280	.4282	.4282	.4282
.4	1.043	1.075	1.0890	1.106
.45	1.240	1.307	1.345	1.513
.5	1.440	1.549	1.617	1.746
.7	2.004	2.042	2.017	1.964
1.	2.078	2.020	2.005	1.997

Table IIc

Convergence of factored approximations to the specific heat C

z	4×4 array	6×6 array	8×8 array	C (exact)
.2	.0684	.0686	.0686	.0686
.4	.6081	.6961	.7473	.8557
.45	.8140	.9808	1.105	1.607
.5	.9901	1.177	1.282	.7155
.7	.6727	.2046	.0320	.1302
1.	-.2004	-.1058	-.0247	.0198

Scaling and a spin bath. The results of the preceding section show that the finite lattice has to be large before the correct critical behavior can be observed, and the costs become prohibitive even with fast enumeration and factorization. The problem would be alleviated if one could replace the naked

edges at the right and top of the array by an appropriate, artificial "spin bath". In the present section we do that by iteration. This is the only one of the constructions of the present paper for which only a heuristic justification can be provided.

We start with a guess of the weights of the partition function of an infinite collection of spins extending to the right and top of a finite lattice, parametrized by the spin at the edge of a large "jaw" (fig. 7). A suitable first guess can be obtained by setting basic blocs next to each other and multiplying the corresponding weights:

$$\Lambda^{\textit{first guess}}_{s_1 \oplus s_2 \oplus s_3 \oplus s_4} = \Lambda^{0}_{s_1} \Lambda^{0}_{s_2} \Lambda^{0}_{s_3} \Lambda^{0}_{s_4}$$

where the $\Lambda^{0}_{s_i}$ are the weights in the parametrization of the basic bloc by s_S (fig. 1).

New basic blocs can be added to the "jaw" through the application of formula (16), until a "small jaw" (fig. 7) is formed. A further basic bloc is then added to provide a new guess for $\tilde{Z}$. To repeat the iteration, a new, improved guess for the weights at the outer jaw is needed and is obtained by similarity from the small jaw.

Indeed, assume that the spins in the big jaw are grouped into pairs, and that the weights attached to a configuration in which two spins in the same pair are misaligned are negligibly small. If the pair is pointing up attach to it a "bloc spin" +1 and if the pair is pointing down attach to it a "bloc spin" -1. The weights attached to the big jaw spin configuration are now

$$\Lambda_{s_1 \oplus s_2 \oplus s_3 \oplus s_4} = \begin{cases} 0 & \textit{if any pair is misaligned} \\ \Lambda_{\tilde{s}_1 \oplus \tilde{s}_2} & \textit{otherwise,} \end{cases}$$

where $\tilde{s}_1, \tilde{s}_2$ are the appropriate m component bloc spin configurations (notice the similarity to the Kadanoff picture [5]).

Now identify the next guess for the weights at the big jaw with the newly computed weights at the inner, small jaw:

$$\Lambda_{\tilde{s}_1 \oplus \tilde{s}_2} = \Lambda_{s_5 \oplus s_6}, \tag{22}$$

i.e., scale up the inner small jaw. This procedure can be repeated until the estimates for $\tilde{Z}$ converge.

One could have expected, by analogy with the Kadanoff picture, that the scaled-up weights should be computed at a temperature T' other than the temperature $T = z^{-1}$ at which we are working (a possibility that is easily programmed and built into the algorithm). However, the choice $T'/T = 1$ is correct at both $T = T_c$ (by analogy with the Kadanoff picture and its generalizations) and at T small (z large) where the bloc-spin assumption is obviously correct; it seems reasonable to keep $T'/T = 1$ at all temperatures.

Formula (21) can be viewed as a prescription for mesh refinement, valid whenever the correlation between spins does not change appreciably over a distance of the order of the distance between spins -- an obvious analogue of the condition under which mesh refinement is allowable in numerical analysis. Indeed, one can reformulate the algorithm in the following way: consider an array of bloc spins and compute the corresponding partition function. Take the left-bottom quarter of the calculation and refine the blocs in that quarter, taking as boundary condition for the refined bloc the weights attached to the bloc spins at its right and top; compute the contribution of the refined corner to the partition function, and repeat the process. This is an analogue of the process carried out for vortices in [3] and can be viewed as a sort of reverse renormalization.

In table III we display some values of φ, U, and C computed with the algorithm just described, with four 2×2 blocs. 2 to 9 iterations are needed for convergence. 3×3 blocs do not substantially improve the results. The plots of

computed vs. exact φ and U are not informative -- on a graph the difference is not visible. The plot of computed vs. exact C is shown in fig. 8. Some improvement over the results displayed in fig. 6 can be discerned. The computed values of C have a clear maximum, at $z = .445 \pm .005$, but the maximum does not reach as high as it does with the renormalization calculation in [6]. The maximum can be sharpened by various ad hoc improvements in the scaling assumption which are not general enough to be worth reporting.

Further work. It is quite clear then the next step in the linkage algorithm is the development of an approximate linkage, i.e., an algorithm analogous to (16),(19) in which small weights are neglected. Such an algorithm, as well as a discussion of its relation to renormalization, will be presented in a subsequent paper together with further applications.

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Note: The programs used above are available from the author.

Table III

φ, U, C computed by the scaling method, four 2×2 blocs

		φ	U	C
$z = .2$	computed	.7341	.4200	.0931
	exact	.7345	.4282	.0686
$z = .4$	computed	.8769	1.113	.8537
	exact	.8794	1.106	.8557
$z = .45$	computed	.9395	1.513	1.092
	exact	.9434	1.394	1.607
$z = .5$	computed	1.016	1.643	.9950
	exact	1.026	1.746	.7155
$z = .7$	computed	1.392	1.995	.1369
	exact	1.404	1.964	.1301
$z = 1.$	computed	1.996	2.014	-.0047
	exact	2.000	1.997	.0198

Bibliography

[1] K.S. Binder, (ed.), *Monte-Carlo methods in statistical physics*, Springer, Berlin (1979).

[2] T.W. Burkhardt and J.M.J. van Leeuwen, (eds.), *Real Space Renormalization*, Springer, Berlin (1982).

[3] A.J. Chorin, Estimates of intermittency, spectra and blow-up in developed turbulence, *Comm. Pure Appl. Math.*, *34*, 853-866 (1981).

[4] A.J. Chorin, Numerical estimates of Hausdorff dimension, *J. Comp. Phys.*, *46*, 390-396 (1982).

[5] L.P. Kadanoff, Scaling laws for Ising models near T_c, *Physics*, *2*, 263-272 (1966).

[6] M. Nauenberg and B. Nienhuis, Renormalization group approach to the solution of general Ising models, *Phys. Rev. Letters*, *33*, 1598-1601 (1974).

[7] T. Niemeijer and J.M.J. van Leeuwen, Renormalization theory for Ising-like spin systems, in C. Domb and M.S. Green, (eds.), *Phase transitions and critical phenomena*, vol. 6, pp. 425-502, Academic, New York (1976).

[8] H.E. Stanley, *Introduction to phase transitions and critical phenomena*, Oxford University Press, New York (1971).

[9] C.J. Thompson, *Mathematical Statistical Mechanics*, Princeton University Press, Princeton, NJ (1972).

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Fig. 6. Factored approximation of the specific heat C as a function of z

Fig. 7. Linkage with scaling

Fig. 8. Approximation of C by linkage and scaling

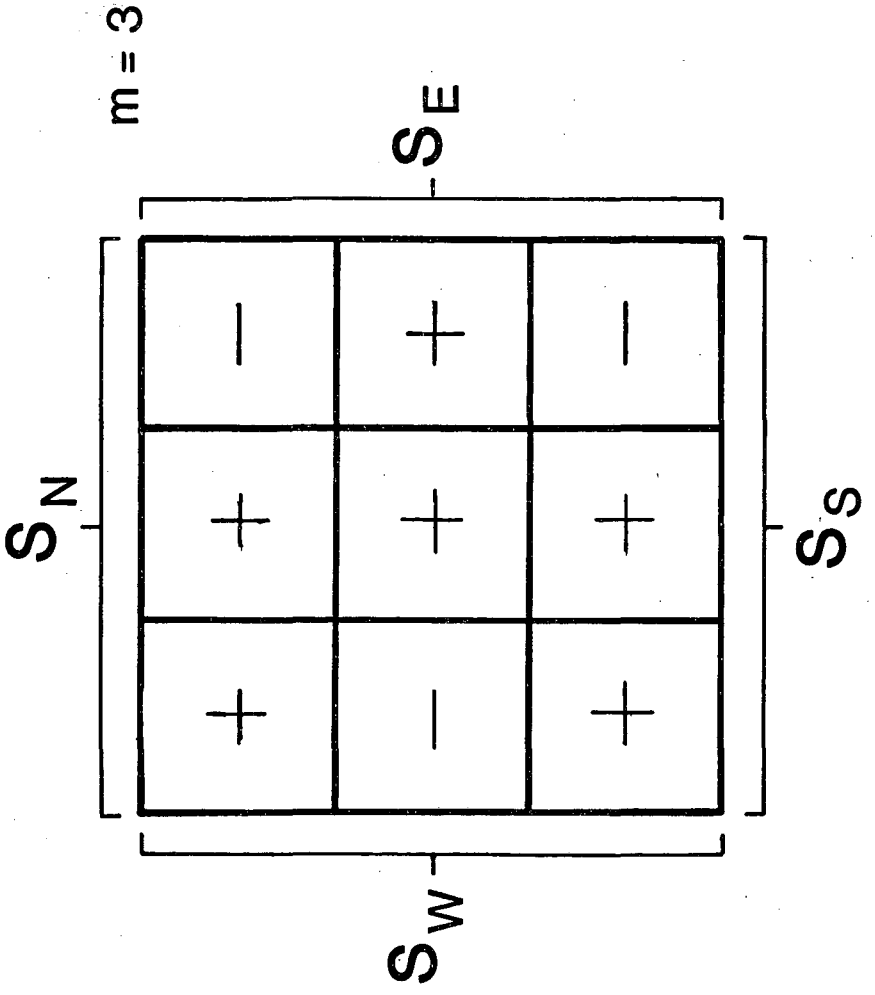

Figure 1

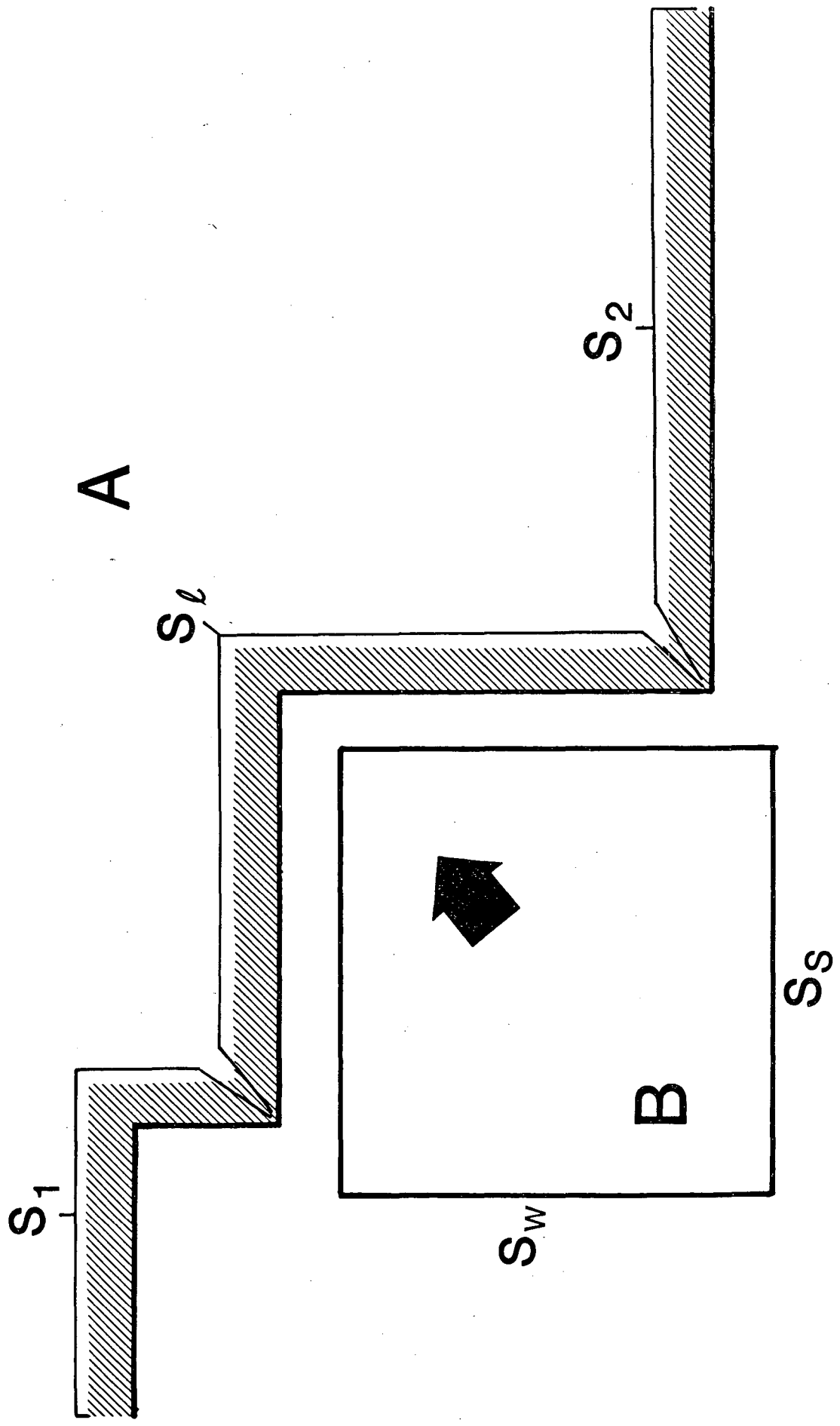

Figure 2

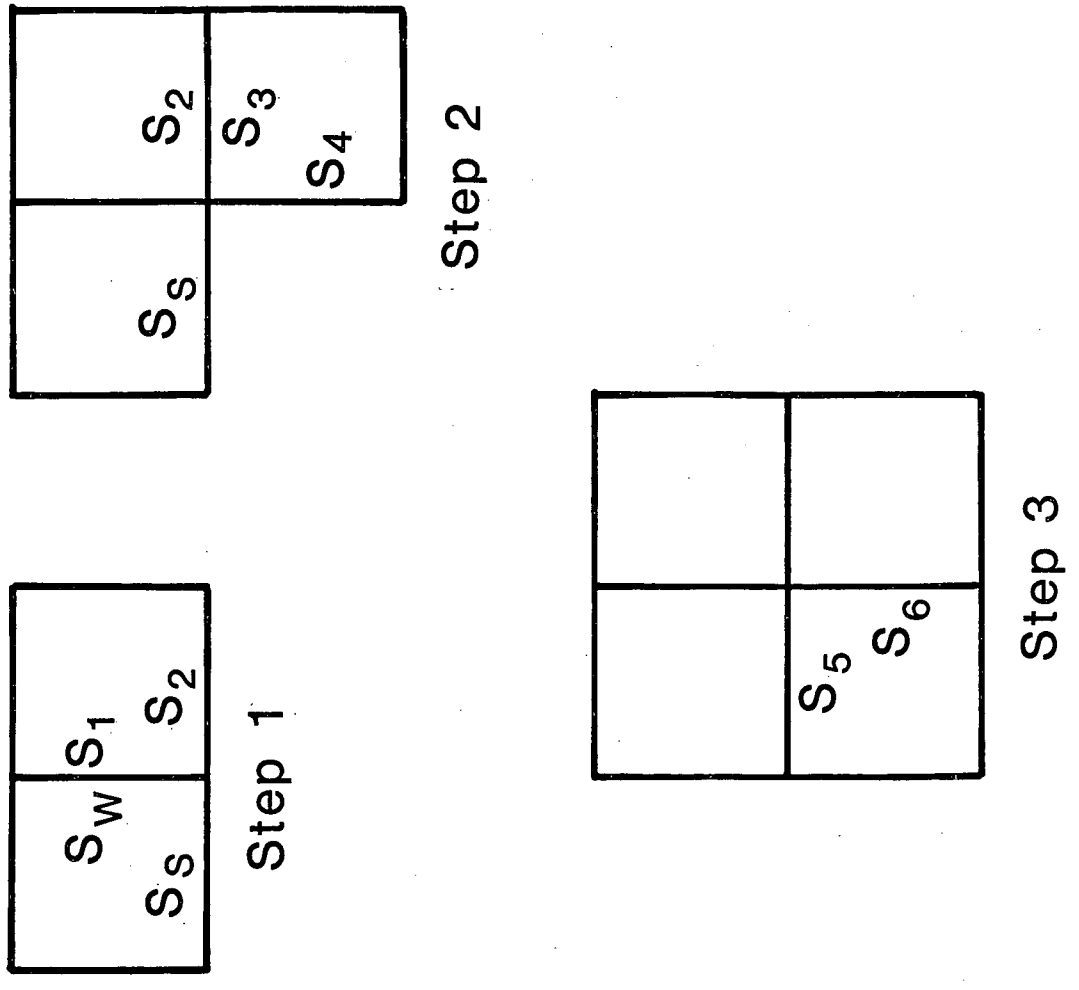

Figure 3

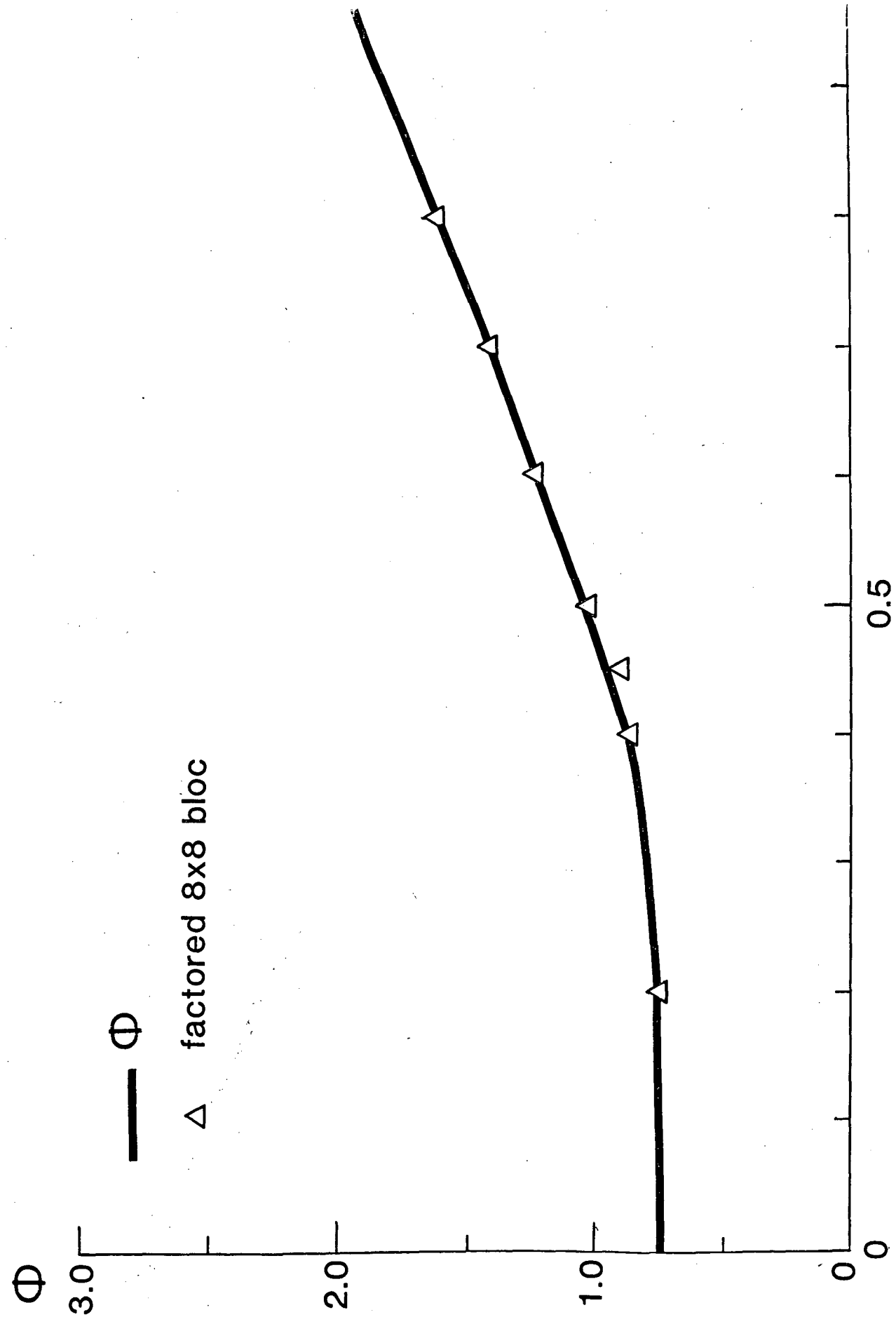

Figure 4

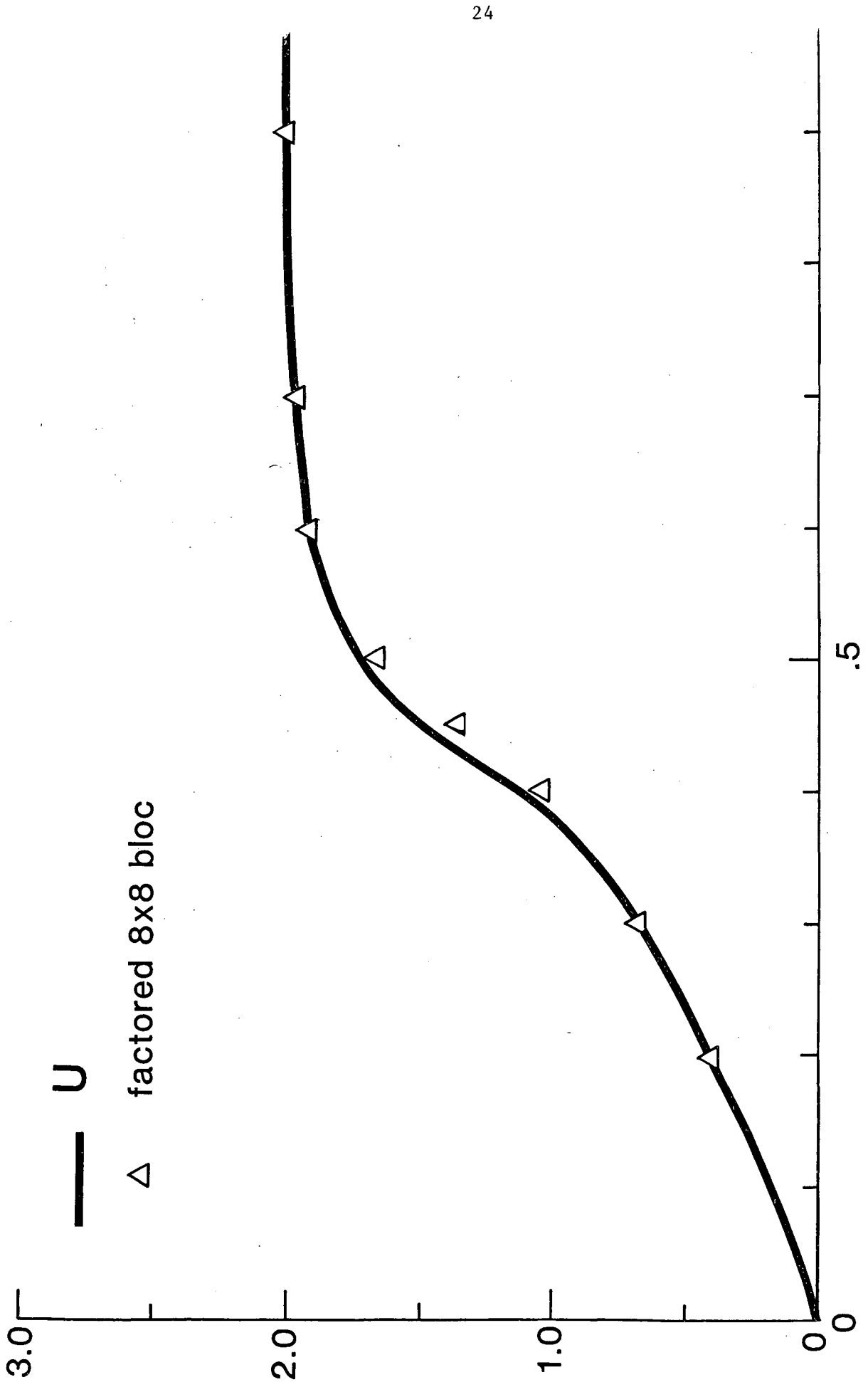

Figure 5

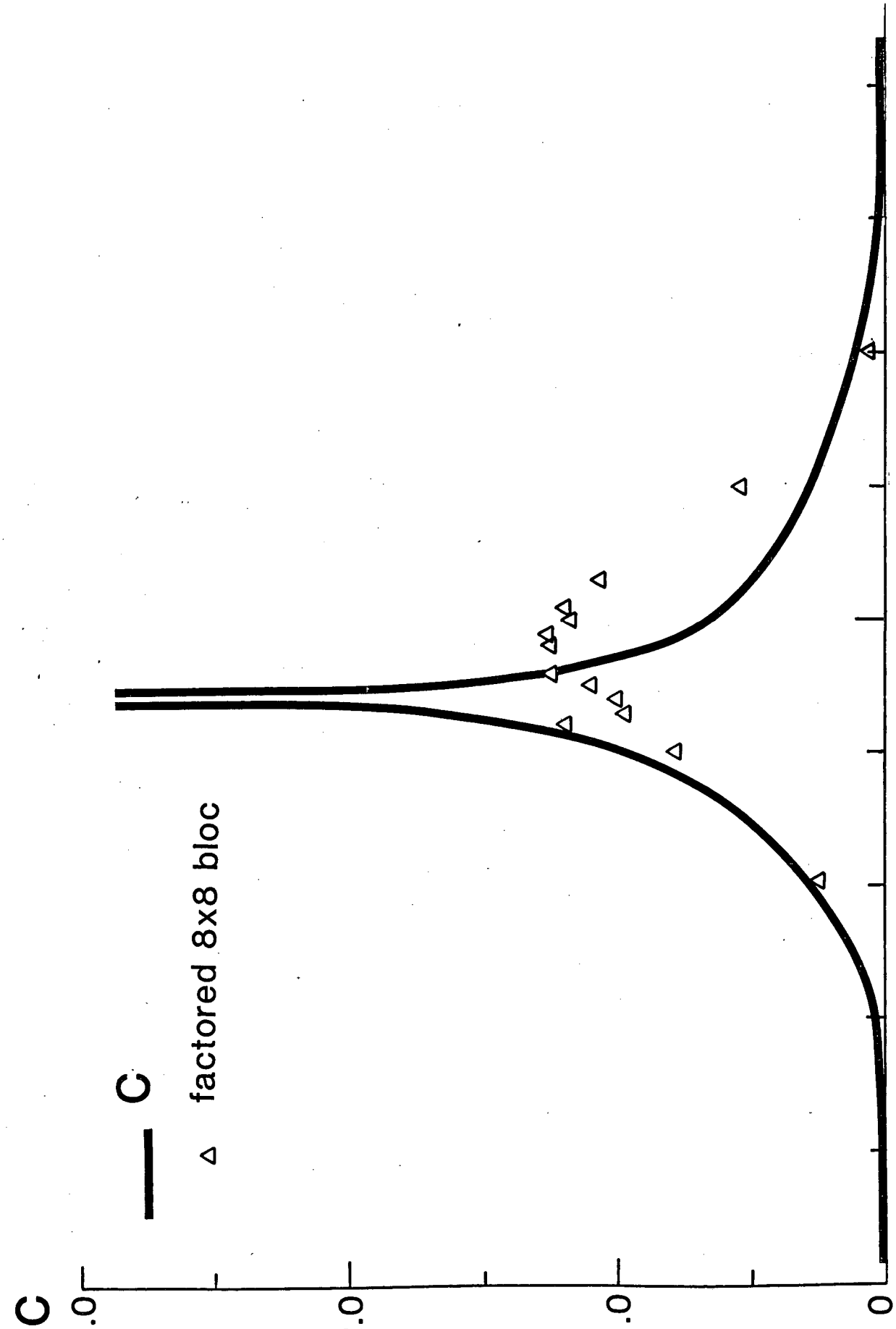

Figure 6

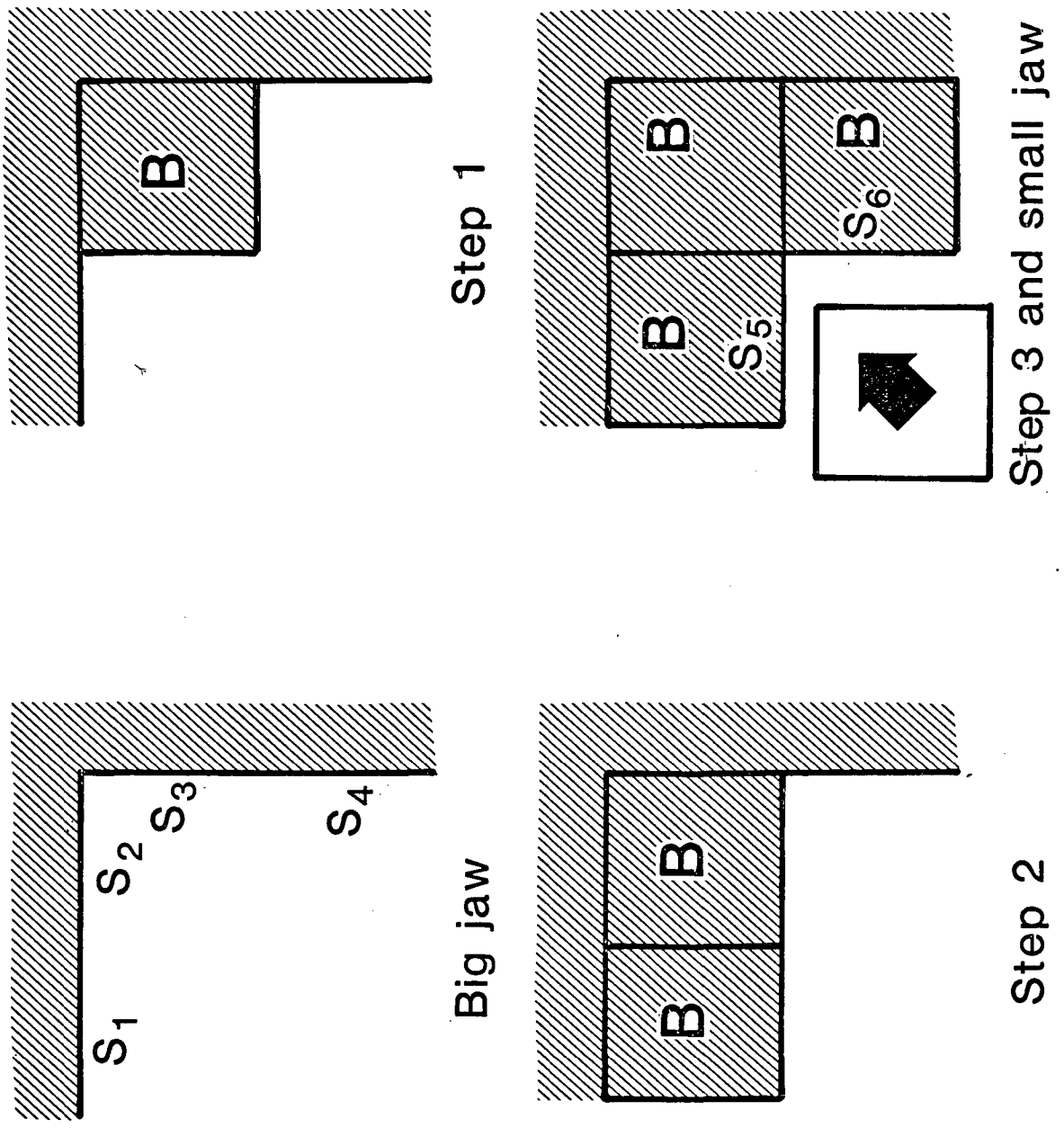
B
Step 1
B
B
S5
S6
B
Step 3 and small jaw
S1
S2
S3
S4
Big jaw
B
B
Step 2

Figure 7

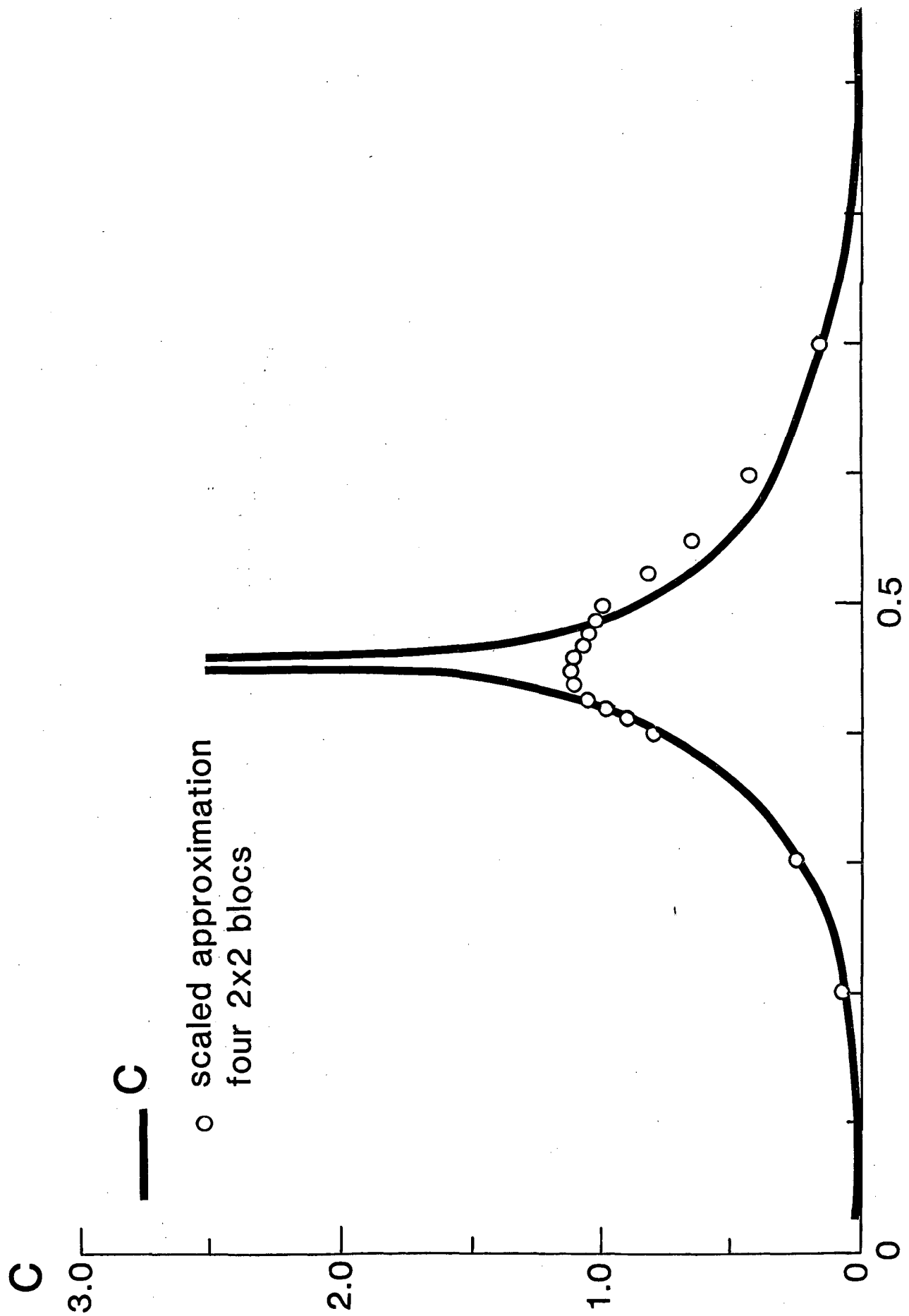

Figure 8

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