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# Solution of Lattice Models by Successive Linkage*

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**Abstract.** A linkage algorithm is presented for evaluating the partition function of a union of finite lattice blocks in terms of the partition functions of the component blocks. 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 number of terms needed to evaluate the partition function for a block of $L$ spins if reduced from $2^L$ to $2^{(\sqrt{L}+\log_2 L)}$); (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 the amount of labor required to evaluate the partition function, the free energy and other thermodynamic quantites 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 blocks to the same quantities evaluated on the component blocks. 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 number of terms to be evaluated is reduced from $2^L$ to $O(L)$; for $L$ Ising spins in the plane, the reduction is from $2^L$ to $2^{(\sqrt{L}+\log_2 L)}$, and in three dimensions, from $2^L$ to $2^{(L^{2/3}+\log_2 L)}$]. This fast enumeration procedure has features in common both with spatial renormalization [2] and with the fast Fourier transform, and does not require any diagonalizations. 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

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their thermodynamic limit (for Ising spins on the line, the thermodynamic limit is reached, after factorization, on a block 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 $(i, j)$, $1 \leqq i \leqq N$, $1 \leqq j \leqq N$, 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 $\varphi_{N\times N}$ per spin 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 $U_{N\times N} = -\dfrac{\partial \varphi_{N\times N}}{\partial z}$, $C_{N\times N} = z^2 \dfrac{\partial U_{N\times N}}{\partial z}$. The Ising model admits a critical point $z_c$, i.e., a non-analytic point of $\varphi$; $\sinh 2z_c = 1$, $z_c = 0.440685\ldots$. 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 block of $m$ spins, which we shall call the basic block. For simplicity, and without loss of generality, we shall write all the formulas in the simple case $m=2$. The basic block 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 block 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 leading spin on the left, and we call the quantities $\Lambda_\pm^0$ the weights attached to the leading spin configuration.

Adjoin to the first block on the left another basic block 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 blocks is

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

where

$$\Lambda_{4,+}=\Lambda_+^0 e^z\Lambda_+^0+\Lambda_+^0 e^{-z}\Lambda_-^0, \tag{8}$$

$$\Lambda_{4,-}=\Lambda_-^0 e^z\Lambda_-^0+\Lambda_-^0 e^{-z}\Lambda_+^0. \tag{9}$$

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 block of 4 spins another basic block and find

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

where

$$\Lambda_{6,+}=\Lambda_+^0 e^z\Lambda_{4,+}+\Lambda_+^0 e^{-z}\Lambda_{4,-},$$

$$\Lambda_{6,-}=\Lambda_-^0 e^z\Lambda_{4,-}+\Lambda_-^0 e^{-z}\Lambda_{4,+};$$

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

$$Z_N=Z^{(1)}Z^{(2)}Z^{(3)}\ldots Z^{(l)},\quad Z^{(1)}=Z^0, \tag{10}$$

with $ml=2l=N$, where $Z^{(i)}$ is the factor by which $Z_{(i-1)l}$ is multiplied when the $i^{\text{th}}$ basic block is added. $Z^{(i)}$ can be viewed as the contribution of the $i^{\text{th}}$ block to the total $Z_N$. Suppose $Z^{(i)}\to\tilde{Z}$, $\tilde{Z}$ independent of $i$. Then

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

thus, $\tilde{Z}$ determines $\varphi$ 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 $\varphi$ 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 block.

From (7)–(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 $i$, $\Lambda_\pm^{(i)}/Z^{(i)}=\frac{1}{2}$ for all $i>1$, and thus for $i>1$,

$$\begin{aligned}Z^{(i)}&=(e^z+e^{-z})(e^z\tfrac{1}{2}+e^{-z}\tfrac{1}{2})+(e^z+e^{-z})(e^z\tfrac{1}{2}+e^{-z}\tfrac{1}{2}),\\&=4\cosh^2 z;\end{aligned}$$

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

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

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 blocks, 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 $\pm 1$. 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 block. There are $2^{m^2}$ spin configurations. Suppose they are generated in some order and tagged by an integer $i$, $1 \leqq i \leqq 2^{m^2}$. 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

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

$s_{SW}$ 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 block is

$$Z_B^0 = \sum_i e^{-zE(i)},$$

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

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

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

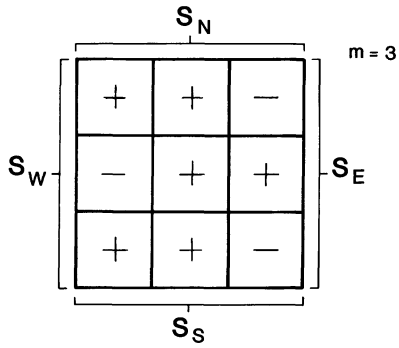


**Fig. 1.** The basic block

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 $\Lambda_s^A$ 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 block $A$ is such that one can attach to it a basic block without gaps or overlaps (Fig. 2). Suppose the leading spin array is written as

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

where $s_l$ contains all the spin sites abutting on the added block, and $s_1, s_2$ are the disjoint, possibly empty, arrays on either side. The partition function for the union of the old block $A$ and the basic block $B$ 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 Eq. (16) are over all relevant boundary configurations, the remaining sum is over all configurations in the block being linked, and the exponential in the middle represents the interactions between the old block and the new block. 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 block, one can start with a small block, and repeatedly adjoin to it blocks 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 $N \times N$ block is, except for negligible factors, determined by the length of the

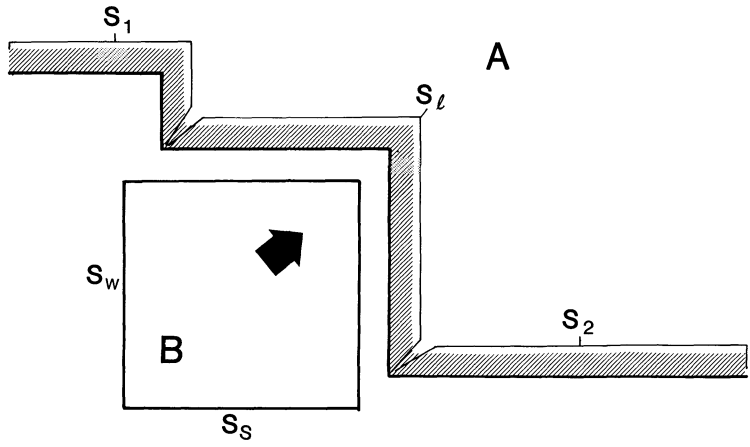


**Fig. 2.** Linkage of a basic block

moving edge of the computed block, i.e., it is of order $2^{O(N)}$, where $N=\sqrt{L}$, $L$ = total number of spins.

The estimate of the amount of labor cannot be sharpened without specifying the size of the blocks $B$ and the linkage strategy. In the case of single spin blocks $B$, of a square $N\times N=L$ and linkage along successive columns, the number of terms to be summed to add a single one-spin block can be readily seen to be $2^N$, and thus the overall number of terms is reduced from $2^L$ to $N^2 2^N = 2^{(\sqrt{L}+\log_2 L)}$.

Another particularly simple case is one in which one constructs $Z$ for the union of only four blocks (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 blocks results in an approximate factorization of the partition function into terms associated with small blocks 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 block 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-block partition function is modified by exponential interaction terms multiplied by suitable probabilities. If the $Z_B$ obtained in successive linkages converge to a limit $\tilde{Z}$, Eq. (18) holds. Note that Eqs. (16) and (18) can be differentiated with respect to $z$ and yield successive approximations $U_{N\times N}\to U$, $C_{N\times N}\to C$.

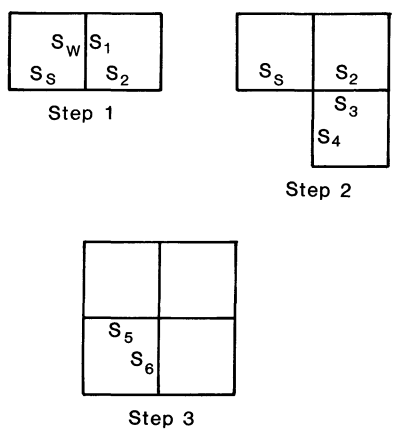


**Fig. 3.** Simple linkage

## 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 $\alpha$ chosen in each part of the calculation so that $l-\alpha \leqq 0$ 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 $\Lambda$'s can become quite large and must be scaled into a reasonable range. If the approximate factorization is used, the scaling of $\Lambda_s^A$ does not change $Z_B$. We assume from now on that these precautions have been taken.

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

Suppose $Z_B^0$, the partition function of the basic block, has been parametrized by $s_S \oplus s_W$,

$$Z_B^0 = \sum_{s_S \oplus s_W} \Lambda_{s_S \oplus s_W}.$$

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

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

where

$$\Lambda^{2\,\text{blocks}}_{s_S \oplus s_2} = \sum_{s_W} \sum_{s_1} \Lambda^0_{s_S \oplus s_W} e^{z(s_W, s_1)} \Lambda^0_{s_1 \oplus s_2}.$$

In the next step

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

where

$$\Lambda^{3\,\text{blocks}}_{s_S \oplus s_4} = \sum_{s_2} \sum_{s_3} \Lambda^{2\,\text{blocks}}_{s_S \oplus s_2} e^{z(s_2, s_3)} \Lambda^0_{s_3 \oplus s_4},$$

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

$$Z_{2m \times 2m} = Z^{4\,\text{blocks}} = \sum_{s_5 \oplus s_6} \sum_{s_S \oplus s_4} \Lambda^{3\,\text{blocks}}_{s_S \oplus s_4} e^{z(s_S \oplus s_4, s_5 \oplus s_6)} \Lambda^0_{s_S \oplus s_4}. \tag{20}$$

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

$$\tilde{Z}_{m \times m} \cong Z^{4\,\text{blocks}} / \Sigma', \tag{21}$$

where

$$\Sigma' = \sum_{s_S \oplus s_4} \Lambda^{3\,\text{blocks}}_{s_S \oplus s_4}.$$

For example, the cost of computing $Z_{4 \times 4}$ is $O(2^{16})$; the cost of computing $Z_{8 \times 8}$ by the algorithm just described is $\sim 4 \cdot O(2^{16})$; the cost of evaluating $Z_{8 \times 8}$ directly,

**Table 1a.** Convergence of $\varphi_{N\times N}$ to the free energy $\varphi$

| $z$ | $\varphi_{4\times 4}$ | $\varphi_{6\times 6}$ | $\varphi_{8\times 8}$ | $\varphi$ (exact solution) |
|---|---|---|---|---|
| 0.2 | 0.7238 | 0.7274 | 0.7291 | 0.7345 |
| 0.4 | 0.8214 | 0.8416 | 0.8507 | 0.8794 |
| 0.45 | 0.8623 | 0.8863 | 0.8991 | 0.9434 |
| 0.5 | 0.9061 | 0.9385 | 0.9563 | 1.026 |
| 0.7 | 1.132 | 1.209 | 1.253 | 1.404 |
| 1.0 | 1.551 | 1.690 | 1.764 | 2.000 |

**Table 1b.** Convergence of $U_{N\times N}$ to the internal energy $U$

| z | $U_{4\times 4}$ | $U_{6\times 6}$ | $U_{8\times 8}$ | $U$ (exact) |
|---|---|---|---|---|
| 0.2 | 0.3140 | 0.3515 | 0.3705 | 0.4282 |
| 0.4 | 0.7067 | 0.8212 | 0.8845 | 1.106 |
| 0.45 | 0.8194 | 0.9681 | 1.056 | 1.513 |
| 0.5 | 0.9324 | 1.118 | 1.233 | 1.746 |
| 0.7 | 1.287 | 1.520 | 1.637 | 1.964 |
| 1.0 | 1.461 | 1.645 | 1.734 | 1.997 |

**Table 1c.** Convergence of $C_{N\times N}$ to the specific heat $C$

| z | $C_{4\times 4}$ | $C_{6\times 6}$ | $C_{8\times 8}$ | $C$ (exact) |
|---|---|---|---|---|
| 0.2 | 0.0681 | 0.0778 | 0.0826 | 0.0686 |
| 0.4 | 0.3549 | 0.4540 | 0.5200 | 0.8557 |
| 0.45 | 0.4604 | 0.6096 | 0.7200 | 1.607 |
| 0.5 | 0.5573 | 0.7362 | 0.8596 | 0.7155 |
| 0.7 | 0.5827 | 0.4981 | 0.4074 | 0.1302 |
| 1.0 | 0.2123 | 0.1274 | 0.0941 | 0.0198 |

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 $8\times 8$ block would otherwise allow. Our evaluation of $Z_{8\times 8}$ with this strategy takes about 2 min on a VAX 780 small computer.

In Tables 1a–c we display $\varphi_{N\times M}$, $U_{N\times N}$, $C_{N\times N}$, computed by formula (28), for $N=4, 6, 8$ as well as the exact values of $\varphi$, $U$, $C$ for some value of $z$. We see that the finite lattice quantities converge very slowly to the thermodynamic limit. In Tables 2a–c, 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 $\varphi$; 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

**Table 2a.** Convergence of factored approximations to the free energy $\varphi$

| $z$ | $4 \times 4$ array | $6 \times 6$ array | $8 \times 8$ array | $\varphi$ (exact) |
|---|---|---|---|---|
| 0.2 | 0.7345 | 0.7345 | 0.7345 | 0.7345 |
| 0.4 | 0.8769 | 0.8784 | 0 8789 | 0.8794 |
| 0.45 | 0.9340 | 0.9379 | 0.9396 | 0.9434 |
| 0.5 | 1.001 | 1.009 | 1.014 | 1.026 |
| 0.7 | 1.355 | 1.384 | 1.395 | 1.404 |
| 1.0 | 1.978 | 1.996 | 1.999 | 2.000 |

**Table 2b.** Convergence of factored approximations to the internal energy $U$

| z | $4 \times 4$ array | $6 \times 6$ array | $8 \times 8$ array | $U$ (exact) |
|---|---|---|---|---|
| 0.2 | 0.4280 | 0.4282 | 0.4282 | 0.4282 |
| 0.4 | 1.043 | 1.075 | 1.0890 | 1.106 |
| 0.45 | 1.240 | 1.307 | 1.345 | 1.513 |
| 0.5 | 1.440 | 1.549 | 1.617 | 1.746 |
| 0.7 | 2.004 | 2.042 | 2.017 | 1.964 |
| 1.0 | 2.078 | 2.020 | 2.005 | 1.997 |

**Table 2c.** Convergence of factored approximations to the specific heat $C$

| z | $4 \times 4$ array | $6 \times 6$ array | $8 \times 8$ array | $C$ (exact) |
|---|---|---|---|---|
| 0.2 | 0.0684 | 0.0686 | 0.0686 | 0.0686 |
| 0.4 | 0.6081 | 0.6961 | 0.7473 | 0.8557 |
| 0.45 | 0.8140 | 0.9808 | 1.105 | 1.607 |
| 0.5 | 0.9901 | 1.177 | 1.282 | 0.7155 |
| 0.7 | 0.6727 | 0.2046 | 0.0320 | 0.1302 |
| 1.0 | 0.2004 | 0.1058 | 0.0247 | 0.0198 |

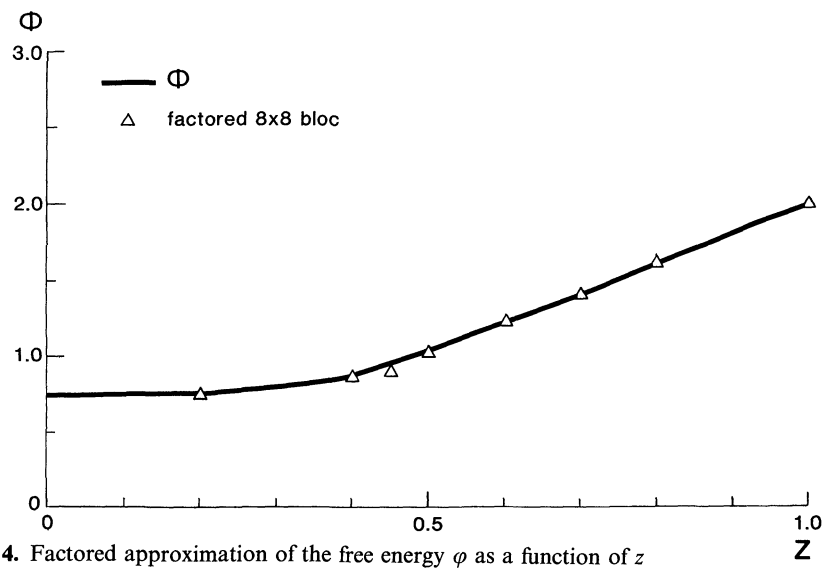


**Fig. 4.** Factored approximation of the free energy $\varphi$ as a function of $z$

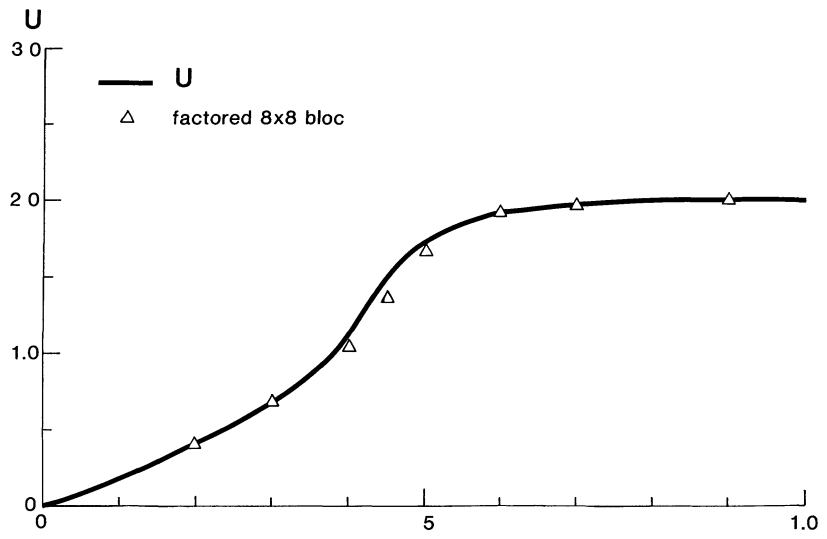


**Fig. 5.** Factored approximation of the internal energy $U$ as a function of $z$

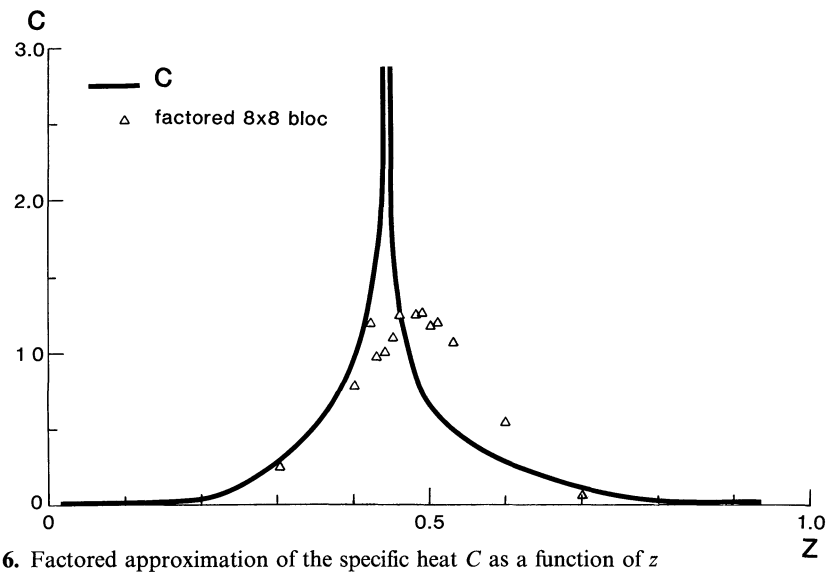


**Fig. 6.** Factored approximation of the specific heat $C$ as a function of $z$

Figs. 4–6. The approximations to $\varphi$ 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 $z=0.41$ and $z=0.51$ – not a bad result for an $8 \times 8$ lattice. Furthermore, the characteristic exponent $\alpha$ is clearly 0, assuming a singularity exists; indeed, the growth of $C$ shows that $\alpha \leqq 0$, and the fact that $C$ remains below the logarithm shows that $\alpha \geqq 0$. These results are not substantially poorer than the numerical renormalization group results in e.g. [6, 7].

## 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 spins at the edge of a large "jaw" (Fig. 7). A suitable first guess can be obtained by setting basic blocks next to each other and multiplying the corresponding weights:

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

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

New basic blocks can be added to the "jaw" through the application of formula (16), until a "small jaw" (Fig. 7) is formed. A further basic block 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 "block spin" $+1$, and if the pair is pointing down, attach to it a "block spin" $-1$. The weights attached to the big jaw spin configuration are now

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

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

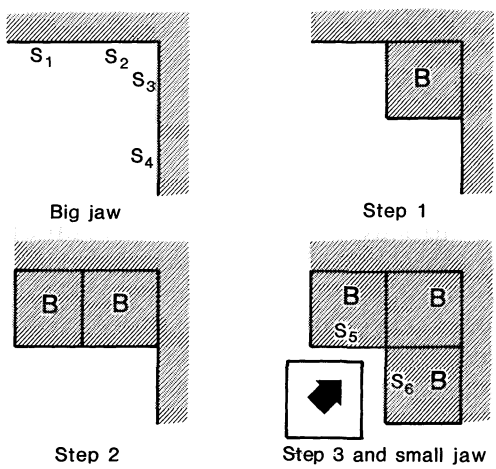


**Fig. 7.** Linkage with scaling

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 block-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 block spins and compute the corresponding partition function. Take the left-bottom quarter of the calculation and refine the blocks in that quarter, taking as boundary condition for the refined block the weights attached to the block 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 3 we display some values of $\varphi$, $U$, and $C$ computed with the algorithm just described, with four $2 \times 2$ blocks. 2 to 9 iterations are needed for convergence. $3 \times 3$ blocks do not substantially improve the results. The plots of computed vs. exact $\varphi$ 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

**Table 3.** $\varphi$, $U$, $C$ computed by the scaling method, four $2 \times 2$ blocks

| | | $\varphi$ | $U$ | $C$ |
|---|---|---|---|---|
| $z=0.2$ | computed | 0.7341 | 0.4200 | 0.0931 |
| | exact | 0.7345 | 0.4282 | 0.0686 |
| $z=0.4$ | computed | 0.8769 | 1.113 | 0.8537 |
| | exact | 0.8794 | 1.106 | 0.8557 |
| $z=0.45$ | computed | 0.9395 | 1.513 | 1.092 |
| | exact | 0.9434 | 1.394 | 1.607 |
| $z=0.5$ | computed | 1.016 | 1.643 | 0.9950 |
| | exact | 1.026 | 1.746 | 0.7155 |
| $z=0.7$ | computed | 1.392 | 1.995 | 0.1369 |
| | exact | 1.404 | 1.964 | 0.1301 |
| $z=1.0$ | computed | 1.996 | 2.014 | 0.0047 |
| | exact | 2.000 | 1.997 | 0.0198 |

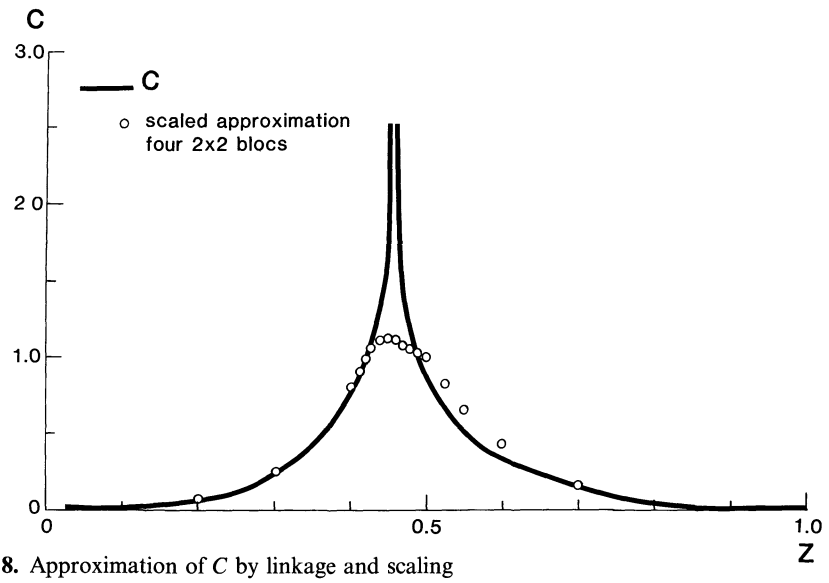


**Fig. 8.** Approximation of $C$ by linkage and scaling

displayed in Fig. 6 can be discerned. The computed values of $C$ have a clear maximum, at $z = 0.445 \pm 0.005$, 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.

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