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An approximate stochastic process for computer simulation of the Ising model at equilibrium

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Abstract. In this work we further develop the stochastic models (SM) method which is an approximate computer simulation technique for treating many-body systems in thermodynamic equilibrium, suggested by Alexandrowicz. The SM method, unlike the commonly used Metropolis method, is not of a relaxation type. Thus, an equilibrium configuration is constructed at once by adding particles to an initially *empty* volume with the help of a model stochastic process. In previous work the transition probabilities (TP) have been expressed as a function of a set of parameters which had to be optimised on the basis of the minimum free energy principle. This choice of TP has the following disadvantages: (1) near to T_c, the critical temperature, the required number of parameters increases and the method becomes impractical; (2) the functional form of the TP is defined in a somewhat intuitive way and, therefore, no criterion exists for *systematically* improving their accuracy. In the present work the TP are defined in a different way and the method is applied as a test to the critical region of the square Ising lattice. First we define the exact TP, which are parameter independent; since their calculation is impractical for a large lattice we also define approximate TP (based on two parameters) which can be improved *systematically*. The saving in computer time, compared with the previous work, (where 10 parameters have been used) is significant, and the accuracy of the free energy is increased by a factor of 4–100. The results for χ, the magnetic susceptibility, are also improved, in particular for $T < T_c$. Using the finite size scaling theory and assuming $\nu = 1$, we estimate at T_c, the exponent γ to be 1.80 ± 0.12. For $T \neq T_c$ the efficiency of the new method is found to be comparable to that of the Metropolis method. At T_c, however, the Metropolis results for χ are exceedingly poor.

1. Introduction

In this work we further develop the stochastic models (SM) method, which is an approximate computer simulation technique for treating many-body systems in thermodynamic equilibrium, suggested by Alexandrowicz (1971, 1972). The SM method, unlike the commonly used Metropolis Monte Carlo method (Metropolis *et al* 1953, Fosdick 1963), is not of a relaxation type. Thus, an equilibrium configuration is constructed at once by adding particles to an initially *empty* volume with the help of a model stochastic process. In contrast to the Metropolis method the probability of the equilibrium configuration is known and this permits one to estimate the entropy (and hence the free energy) directly. The SM method procedure is naturally carried out in the framework of the (μ, V, T) ensemble but can also conveniently be performed in the (N, P, T) ensemble, which in general fits better to the experimental conditions than the (N, V, T) ensemble. Because of this *ab initio* type of construction the configurations sampled are statistically uncorrelated and therefore much smaller

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samples are required with the SM method than with the Metropolis procedure. The SM method has been recently applied to the square and cubic Ising lattices and good results have been obtained (Meirovitch and Alexandrowicz 1977a). In the present paper we shall use the abbreviation MA for that reference. The method was also applied to a fluid model consisting of hard cubic molecules with an attractive potential (Alexandrowicz and Mostow 1972) and to a lattice version of the Maier–Saupe model for nematic liquid crystals (Meirovitch 1977b). In all these works the transition probabilities (TP) of the stochastic process have been expressed as a function of a set of parameters which had to be optimised on the basis of the minimum free energy principle. This choice of TP has the following disadvantages: (1) near to T_c, the critical temperature, where long-range correlations exist, the required number of parameters increases and the method becomes impractical (for the square Ising lattice, for example, a set of 10 parameters has been used by MA); (2) the functional form of the TP is defined in a somewhat intuitive way and, therefore, no criterion exists for improving their accuracy sytematically.

In the present work we use the construction procedure of the SM method but define the TP in a novel way, and apply the method as a test to the critical region of the square Ising lattice. Firstly we define the exact TP which are parameter independent. Since their calculation is impractical for large lattices we also define two kinds of approximate TP, based on one and on two parameters. These approximations to the exact TP, in contrast to those of previous work, can be improved systematically. The present results (obtained with the second approximation) are compared with results obtained by MA with the SM and the Metropolis methods and the efficiency of the three methods is discussed.

2. The SM method construction procedure

We shall now describe briefly the SM method lattice construction procedure as applied to the square Ising lattice with $N = L \times L$ spins; more details appear in MA. We denote by σ_k the spin variable at the lattice site k, where σ_k has two possible values: $+1$, -1. The interaction is only betweeen nearest-neighbour spins and it is of a ferromagnetic type (the coupling interaction constant $J > 0$). The microscopic energy E_i and magnetisation M_i of a particular configuration are given respectively by

$$E_i = -J \sum_{\substack{kl \\ (\mathrm{nn})}} \sigma_k \sigma_l \tag{1}$$

$$M_i = N^{-1} \sum_{k=1}^{N} \sigma_k \tag{2}$$

where (nn) denotes nearest neighbours. The canonical ensemble probability (Boltzmann probability) P_i^{B} of configuration i at the absolute temperature T is defined by

$$P_i^{\mathrm{B}} = Z^{-1} \exp(-E_i / k_{\mathrm{B}} T) \tag{3}$$

where Z denotes the partition function and k_{B} is the Boltzmann constant. The construction of a lattice configuration is carried out as follows: one begins with an empty lattice and fills the first row with spins which are distributed at random. Subsequently, the orientation of the spins on the lattice is fixed step by step by a

Monte Carlo lottery according to transition probabilities which depend on a given set of parameters x and on the L spins determined in the previous steps of the process. Once the construction of the lattice configuration i has been accomplished its microscopic energy and its probability $P_i(x)$ beome known. $P_i(x)$ is the product of the N TP with which the spins have been chosen. In this way a probability distribution (PD) is defined on phase space and a free energy functional $F(x)$ can also be defined. The minimum free energy principle states that $F(x)$ is never smaller than the exact free energy obtained with the Boltzmann probability P_i^B (equation (3)). The problem is to find the best approximate PD in the sense of this principle. Sampling n configurations with $P(x)$ enables one to estimate $F(x)$ by

$$F_n(x) = n^{-1} \sum_{t=1}^{n} (E_{i(t)} + k_B T \log P_{i(t)}(x)) \tag{4}$$

and then seek the optimal set of parameters x^* giving the minimum value to $F_n(x)$. For this value one computes the average energy and the other lattice quantities of interest.

In the present work we use the lattice construction procedure described above, but define the TP in a novel way. In the next section we first define the exact TP, i.e. those which lead to the Boltzmann distribution (equation (3)). Since they are parameter independent, no optimisation of equation (4) is required. The calculation of the exact TP, however, is impractical for large lattices and thereafter we describe two approximate TP based on one and on two parameters.

3. The transition probabilities

3.1. The exact transition probabilities

Assume that we are at the kth step of the SM construction, i.e. the orientation of $k-1$ spins has already been specified, and we want to specify the spin orientation σ_k at site k. The exact TP is proportional to the conditional partition function $Z(\sigma_k, I_k)$,

$$Z(\sigma_k, I_k) = \sum_{\text{all } i} \exp\{-[E(i) + E(I_k, J_i) + E(\sigma_k, \sigma')]/k_B T\}. \tag{5}$$

The index i in (5) runs over all 2^{N-k} possible spin configurations on the still empty lattice (sites $k+1, \ldots, N$) which can be obtained in future steps of the process (figure 1). These yet undetermined spins should be distinguished from the $k-1$ already fixed ones and we therefore call them the future spins; correspondingly, configuration i defined above will be called future configuration i. $E(i)$ is the microscopic energy of the future configuration i. I_k is the *row* configuration of the last L spins added to the lattice (on sites $k-L, \ldots, k-1$). For a given future configuration i, J_i denotes the row configuration of the $L-1$ future spins on sites $k+1, \ldots, k+L-1$ (see figure 1). $E(I_k, J_i)$ stands for the interaction energy between the two neighbour row configurations I_k and J_i. $E(\sigma_k, \sigma')$ denotes the interaction energy of σ_k with its four nearest neighbours σ'. The normalised *exact* TP is therefore

$$p(\sigma_k | I_k) = Z(\sigma_k, I_k)[Z(\sigma_k, I_k) + Z(-\sigma_k, I_k)]^{-1} = [1 + Z(-\sigma_k, I_k)/Z(\sigma_k, I_k)]^{-1}. \tag{6}$$

It should be pointed out that the fact that $p(\sigma_k | I_k)$ do not depend on *all* the $k-1$ already fixed spins, but only on I_k, is due to the nearest-neighbour type of interaction

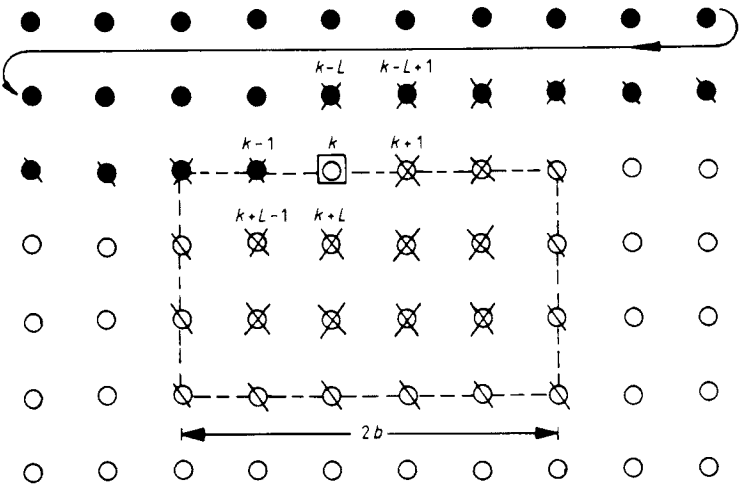

Figure 1. An illustration of the kth step of the spiral construction of the square Ising lattice. Full circles denote lattice spins already specified in the previous steps of the process while open circles denote the still empty lattice sites. The full curve indicates the present 'spiral' boundary conditions. The broken lines define a rectangle of $2b \times (b+1)$ lattice sites with $b = 3$, for the first approximation. The crossed full circles (⊗) and the slashed full ones (⦸) denote groups A and B respectively, while group A', and group B' of the surface future spins are denoted by the crossed open (⊠) and slashed open circles (⦸) respectively. The rest of the open circles denote group C. These groups are defined in the text.

of the model; adding, for example, second neighbour interactions, would make $p(\sigma_k|I_k)$ a function of the $2L$ last determined spins. It is easy to prove that a lattice configuration i is sampled with its Boltzmann probability P_i^B (equation (3)) if constructed according to the exact TP defined above; in this case there is no need of optimisation since the TP are free of parameters. However, calculation of the 2^L exact TP is very time consuming for a large lattice and requires a huge computer memory. In order to make the calculation feasible we therefore introduce, in what follows, two kinds of approximate TP.

3.2. The first approximation

The first kind of approximate TP is based on dividing the L spins $\sigma_{k-L}, \ldots, \sigma_{k-1}$ into two groups. The first group, called group A, contains the $2b$ closest spins to site k (on sites $k-L, \ldots, k-L+b$ and $k-b+1, \ldots, k-1$), where the effective distance of a spin from site k is defined by its shortest distance from site k measured on *empty* lattice bonds (see discussion by MA). These spins are denoted by the crossed full circles (⊗) in figure 1 and their effect is taken into account in an exact way. The $L-2b$ spins placed on the more distant sites $(k-L+b+1, \ldots, k-b)$ constitute group B (slashed full circles (⦸) in figure 1) and they are treated approximately by using a mean field parameter t. We define a $2b \times (b+1)$ rectangle (denoted by broken lines in figure 1), with $2b^2+b$ empty lattice sites, which consists of two groups of future spins: group A' of the inner future spins (crossed open circles (⊠) in figure 1) and group B' of the surface future spins (denoted by slashed open circles (⦸) in figure 1). The group of future spins located outside the rectangle is denoted by C. We define an approximate conditional partition function $Z(\sigma_k, I_k, b, t)$, related to the rectangle,

and the corresponding TP are obtained by equation (6), where $Z(\sigma_k, I_k, b, t)$ replaces $Z(\sigma_k, I_k)$ (equation (5)). $Z(\sigma_k, I_k, b, t)$, unlike $Z(\sigma_k, I_k)$, takes into account exactly *only* the spins of groups A and A', whereas the effect of groups B, B' and C is approximated as follows: each future spin σ of the surface group B' interacts with its neighbour spins of groups A and A'; however, instead of also interacting with its neighbours of group C, σ interacts with the mean field parameter t, contributing to $Z(\sigma_k, I_k, b, t)$ factors of the type $\exp(Jt\sigma/k_B T)$. The parameter t represents the average effective magnetisation per spin of group C and therefore falls in the range $[-1, +1]$. We define the sign of t to be the same as that of the magnetisation of group B; therefore the sign of t is a function of k and might change during the SM construction process, in contrast to $|t|$ which is constant for all the TP. $|t^*|$, the absolute value of the optimal parameter, is a function of both b and T and is determined by minimising $F_n(t)$ (equation (4)). Below the critical temperature, T_c, where long-range order exists, $|t^*|$ is expected to be relatively large; above T_c we expect $|t^*| \sim 0$. Obviously, as b is increased the approximation improves and the effect of t weakens; determination of t^* in that case therefore requires higher statistical accuracy, which means a larger sample size. The approximation is valid as long as b is sufficiently large relative to the correlation length ξ. Therefore, close to T_c, where ξ diverges, large values of b should be used which makes the calculation impractical.

3.3. The second approximation

We now describe a method which enables one to enlarge the dimensions of the rectangle defined in the previous section, but control the number of distinct TP. For this we divide the L spins $\sigma_{k-L}, \ldots, \sigma_{k-1}$ into three groups. The first one (A) consists of the $2b$ nearest spins to site k (figure 2). The second group (B) contains the $2(a-b)$

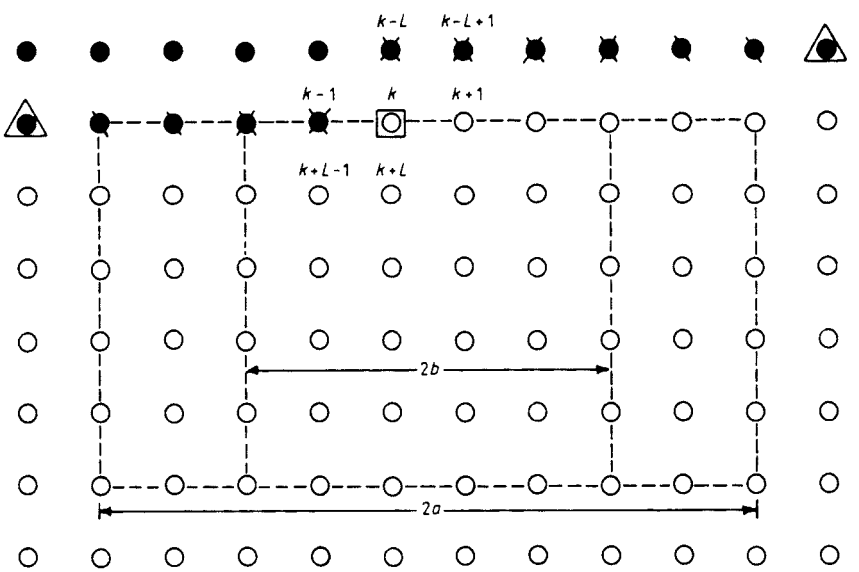

Figure 2. An illustration, similar to figure 1, for the second approximation. The crossed (⊗) and slashed (⊘) full circles denote groups A and B respectively. The full circles enclosed by triangles ⧋ denote group C. These groups are defined in the text. The broken lines define the inner and the outer rectangles of $2b \times (a+1)$ and $2a \times (a+1)$ lattice sites respectively, with $b = 3$ and $a = 5$.

farther placed spins with $b+1<r<a+1$, where r is the distance of a spin from site k and $a>b$. The rest of the spins (with $r>a+1$) constitute the third group (C). Correspondingly we define two rectangles of dimensions $2b\times(a+1)$ and $2a\times(a+1)$ (figure 2), and a conditional partition function $Z(\sigma_k, I_k, a, b, c, t, f)$ related to them. c and f are parameters which will be defined below. The effect of the spins of group C is approximated in this function as before, by using a mean field parameter t, i.e. all future spins on the surface of the larger rectangle $[2a\times(a+1)]$ interact with t as has been explained in the previous section.

The effect of the spins of group A is treated in an exact way (as in the first approximation) by taking into account the contribution of all future spins of the inner rectangle $2b\times(a+1)$. It should be pointed out that the future spins on the side boundaries of this rectangle interact with all their neighbour spins, including those which belong to the larger rectangle. These two groups of spins contribute a factor 2^{2b+1} to the total number of TP; obviously, treating the spins of group B in an exact way would increase this number by a factor of $2^{2(a-b)}$. In order to control this number for large values of $a-b$ we define the following approximation. We assume (as was assumed by MA) that the effect of a spin of group B decreases with distance r from site k as r^{-f}, where f is a positive decay parameter. This enables us to define the normalised spin charges σ_R and σ_L for the configuration j of $a-b$ spins from the right and left sides of site k respectively.

$$\sigma_R(j)=\left(\sum_{m=b+2}^{a+1} m^{-f}\sigma_{k-L+m-1}\right)\left(\sum_{m=b+2}^{a+1} m^{-f}\right)^{-1}$$

$$\sigma_L(j)=\left(\sum_{m=b+2}^{a+1} m^{-f}\sigma_{k-m+2}\right)\left(\sum_{m=b+2}^{a+1} m^{-f}\right)^{-1}. \tag{7}$$

In these summations individual spins are multiplied by the decreasing function m^{-f} where m is the distance (in lattice steps) from site k. σ_R (and σ_L) has 2^{a-b} distinct values, which fall in the range $[-1, +1)$. We divide this range into c equal segments and find for each one of them the configuration j with $\sigma_R(j)$ (or $\sigma_L(j)$) closest to the centre of the segment. Each of these c configurations is taken to represent all configurations j with value σ_R (or σ_L) within the limits of the segment. In this way the spins of the second group contribute a factor c^2 to the total number of TP irrespective of their number $2(a-b)$. Clearly, the larger c, the better the approximation.

3.4. Details of the computation of the TP

In the present work we carry out calculations using the second approximation with $b=5$, $a=14$ and $c=12$. These values determine the computer program and are not changed during the optimisation procedure. In general the larger a, b and c, the better the approximation. However, the choice of these parameters is mainly dictated by computer speed and memory. We found, for example, that for the above values of a and b increasing c from 10 to 12 (which is a trivial change in the program) lowered the free energy at T_c by not more than about 2×10^{-6}. The conclusion is that for a better approximation either a or b should be increased but not c. In the present calculation we determined the width of the rectangle to be 12 lattice sites rather than 14, which means that altogether 322 future spins are taken into account in the calculation of the TP. In order to make this calculation feasible we first compute the contributions of separate blocks of future spins and later combine them together. The

TP (102 400 in the present work) are calculated and stored in computer memory prior to the simulation process. Using the Q compiler on the IBM 370/165 about 3 minutes are required for the calculation of these TP and the construction of a 120×120 lattice takes about 0.5 s.

4. Results and discussion

The essential part of the work is the determination of the optimal parameters t^* and f^* giving a minimum to the free energy functional estimator $F_n(t, f)$ (see equation (4)). Using the optimal parameters the average energy $E_n(t^*, f^*)$, magnetisation $M_n(t^*, f^*)$ and the order parameter $|M_n(t^*, f^*)|$ are calculated. The equation for the order parameter is

$$|M_n(t^*, f^*)| = n^{-1} \sum_{i=1}^{n} |M_{i(t)}|. \tag{8}$$

The specific heat C and the isothermal susceptibility per spin χ are obtained from the variances of E and M respectively, using known thermodynamic relations (see MA).

The results of the present work for the various thermodynamic quantities in the critical region are summarised in table 1, together with the corresponding values obtained by the accurate analytical solution and with approximate expressions based on series expansion. For comparison we give also results obtained by MA with the SM and the Metropolis methods. The exact correlation length (Fisher 1967) and the optimal values of the parameters, t^* and f^* are presented in the three bottom rows of the table. For $K \neq K_c$ ($K = J/k_B T$ is the reciprocal temperature and K_c its critical value) the present results have been calculated from samples of 5000 configurations whereas for the critical temperature, the sample size has been increased to 8000. In order to estimate the statistical error, for each temperature we have carried out several tests based on different random number sequences. The uncertainties in the results appearing in the table take into account the uncertainty in the determination of the optimal parameters. Let us discuss first the results for $K \neq K_c$. The results of the present work for the free energy F are substantially better than those obtained with the SM method by MA. The improvement is especially significant in the cold region ($K > K_c$) where accuracy of about $10^{-4}\%$ is achieved, which is 100 times larger than that obtained by MA. In the hot region ($K < K_c$) the accuracy in F is increased by a factor of 25–4, compared with MA, changing from 10^{-4}–$3 \times 10^{-3}\%$ in going from $K = 0.40$ to $K = 0.43$ respectively. From the point of view of the minimum free energy principle this means that the probability distributions defined by the present TP are better than those defined by the SM method (MA) and the results here for the other thermodynamic quantities are therefore also expected to be more accurate. It should be pointed out that relatively accurate estimates for the entropy, and hence for the free energy, can also be obtained with the Metropolis method by employing a method suggested recently (Meirovitch 1977a). However, the best accuracy for F obtained so far with this method for the square lattice gas model is 10^{-1}–$10^{-2}\%$, which is significantly lower than that of the present work (Meirovitch and Alexandrowicz 1977b). Very good agreement with the theoretical values is obtained with the present method for the energy E and the long-range order $|M|$, where the largest discrepancy 0.4% occurs for the energy at $K = 0.43$. A comparable accuracy for these quantities has been obtained by MA with the SM and the Metropolis methods. In view of the

Table 1. Results for the square Ising lattice: free energy F, energy E, long-range order $|M|$, specific heat C and magnetic susceptibility χ obtained with the present transition probabilities, and with theoretical methods (analytical and series expansion). Results obtained by MA with the SM method (denoted SM) and with the Metropolis method (10^4 lotteries per spin) are also presented. K is the reciprocal temperature $K = J/k_B T$ and $K_c = 0.44068\ldots$ is its critical value (Onsager 1944), L is the lattice size $N = L^2$, ξ is the exact correlation length (Fisher 1967), $|t^*|$ and f^* are the optimal values of the mean field and decay parameters respectively. The errors in the last digits appear in parentheses; for example: 0.879(23) means 0.879 ± 0.023 (the error is defined in the text). The exact results of $K \neq K_c$ are calculated using formulae for the infinite lattice (Newell and Montroll 1953). At $K > K_c$ χ is calculated using a Padé approximant (Essam and Fisher 1962) and at $K < K_c$ with the approximate high-temperature expansion formula (Sykes *et al* 1972). At K_c the accurate values of E and C are calculated from the analytical solution for a finite lattice (Ferdinand and Fisher 1969). Not available theoretical values are marked NA.

	K	0.40	0.41	0.42	0.43	K_c	K_c
	L	120	120	120	150	40	64
$-F/Nk_BT$	Present	0.879 363(1)	0.890 699(1)	0.902 631(1)	0.915 232(1)	0.929 826(3)	0.929 721(2)
	Theoretical	0.879 364	0.890 703	0.902 639	0.915 260	0.930 095	0.929 852
	SM	0.879 34	0.890 65	0.902 56	0.915 12	0.929 58	0.929 47
$-E/NJ$	Present	1.105(1)	1.162(1)	1.224(1)	1.295(1)	1.414(4)	1.413(4)
	Theoretical	1.106	1.163	1.226	1.300	1.430	1.424
$\|M\|$	Present	0.052(1)	0.065(1)	0.090(1)	0.126(2)	0.55(2)	0.53(2)
	Theoretical	NA	NA	NA	NA	NA	NA
C/Nk_B	Present	0.85(1)	0.97(2)	1.14(2)	1.43(6)	1.66(2)	1.80(2)
	Theoretical	0.86	1.00	1.20	1.53	1.95	2.18
	SM	0.85	1.00	1.28	1.65	1.98	2.34
	Metropolis	0.82	1.02	1.17	1.55	1.70	2.23
$x\|N$	Present	60(2)	97(4)	185(7)	550(30)	560(30)	1350(60)
	Theoretical	62	102	204	647	NA	NA
	SM	60	100	180	450	620	1440
	Metropolis	50	100	195	350	24	300
ξ		6.0	8.0	11.9	23.2	NA	NA
$\|t^*\|$		0.013	0.018	0.024	0.041	0.126	0.158
f^*		3.1	3.1	2.5	1.9	1.9	1.9

	K	K_c	K_c	K_c	0.455	0.46	0.47
	L	76	90	120	120	120	120
$-F/Nk_BT$	Present	0.929 702(2)	0.929 689(1)	0.929 677(1)	0.951 042(1)	0.958 871(1)	0.974 958(1)
	Theoretical	0.929 806	0.929 774	0.929 740	0.951 043	0.958 871	0.974 958
	SM	NA	0.929 44	0.929 41	0.950 92	0.958 75	0.974 88
$-E/NJ$	Present	1.412(3)	1.413(3)	1.414(1)	1.549(1)	1.580(1)	1.634(1)
	Theoretical	1.422	1.421	1.419	1.550	1.581	1.634
$\|M\|$	Present	0.52(2)	0.52(2)	0.53(3)	0.788(1)	0.814(1)	0.852(1)
	Theoretical	NA	NA	NA	0.788	0.815	0.852
C/Nk_B	Present	1.85(2)	1.87(2)	2.00(3)	1.38(2)	1.24(2)	1.06(1)
	Theoretical	2.27	2.35	2.50	1.40	1.25	1.05
	SM	NA	2.43	2.56	1.40	1.25	1.10
	Metropolis	2.60	2.25	2.50	1.45	1.17	1.01
χ/N	Present	1750(80)	2500(100)	4300(200)	8.6(4)	5.6(3)	2.75(8)
	Theoretical	NA	NA	NA	10	6	2.8
	SM	NA	2700	4800	5	3.4	2.0
	Metropolis	1850	400	350	10	4.7	2.7
ξ		NA	NA	NA	8.8	6.6	4.4
$\|t^*\|$		0.152	0.164	0.165	0.384	0.403	0.458
f^*		1.9	1.9	1.9	3.25	3.25	3.2

highly accurate results obtained here for both F and $|M|$ one would expect to obtain accurate estimates for the pressure P in lattice models for fluids treated with the present method in the framework of the grand canonical ensemble. This is because P can be expressed by

$$P = \rho(\mu - F/N) \tag{9}$$

where μ is the chemical potential, N is the number of particles and ρ is the density, which corresponds to the magnetisation M of the Ising model (Fisher 1967). The magnetic susceptibility and the specific heat C are the two thermodynamic quantities most sensitive to the approximation used. For $K \neq K_c$ the results for C, obtained by the three methods, agree well with the exact values where the deviations do not exceed 8%. The poor results obtained for χ with the SM method (MA) in the cold region (accuracy of 25–50%) are substantially improved in the present work, where accuracy of 2–12% is achieved respectively. For $K < K_c$ a significant improvement in χ is obtained for $K = 0.43$ (accuracy $\sim 15\%$) whereas for the other temperatures the results of the three methods are about the same. It should be noted that the results for χ obtained with the present method and the SM method (MA) always underestimate the correct values.

The fact that the results of the present method in the cold region are much better than those of the SM method (MA) stems mainly from the more correct definition of the mean field parameter t in the present TP. In the hot region, however, where the long range order vanishes, the effect of t significantly weakens, which is expressed by an improvement in the results of the SM method (MA). We have confirmed this explanation by changing the definition of t in the present TP to the way it was defined in equations (12) and (15) of MA. The values for F obtained with the new definition were indeed much higher than those of the present work, and close to the results obtained with the SM method by MA. In this context it should be also pointed out that even with the TP of the present work the results for χ for the hot region are better than those of the cold region. This is demonstrated, for example, at reciprocal temperatures $K = 0.455$ and $K = 0.41$ which have approximately the same correlation length ξ but the values of χ deviate from the exact ones by 12% and 5% respectively.

At K_c we present results for 5 lattices, from $L = 40$ to $L = 120$, using a larger sample size of 8000 configurations; the uncertainty in the results, however, is still larger than that obtained for $K \neq K_c$ due to the larger thermodynamic fluctuations at K_c. We compare the results with the exact solution for a finite lattice with periodic boundary conditions (PBC) (Ferdinand and Fisher 1969). It should be pointed out that the present screw boundary conditions (SBC) differ from the PBC, mainly because the first and last rows of the lattice do not interact. For small lattices, therefore, the PBC give significantly higher statistical weight than the SBC to configurations where the magnetisation of these two rows is of the same sign. One would therefore expect to obtain larger values for $|M|$, C and χ and lower values for E with PBC than with the present calculations. The results for E and C confirm this expectation. The effect of the boundary conditions should be most significant for the smallest lattice $L = 40$; indeed, the corresponding value of F shows the largest deviation from the exact value. As is expected, this deviation decreases with increasing lattice size. Our results for F are much lower (and hence better) than those obtained with the SM method (MA). However, unlike for $K \neq K_c$, it is impossible to determine their accuracy since no exact solution exists for a finite lattice with SBC. As has been already pointed out the results for C of the present calculation are smaller than the exact ones. In view of

the analytical solutions (Onsager 1944, Ferdinand and Fisher 1969) one would expect them to approximately satisfy a linear dependence on $\log L$. We have made the best fit of these results to such a function and obtained the expression

$$C/Nk_B = 0.32 \log L + 0.46 \tag{10}$$

which gives the values 1.64, 1.79, 1.84, 1.90, 1.99 for the five lattices $L = 40$, 64, 76, 90, 120 respectively; these results are in a good agreement with the corresponding values of C obtained with the present method. It should be noted however that the factors 0.32 and 0.46, which appear in equation (10), differ from the corresponding pairs 0.495 and 0.198 and 0.495 and 0.188 obtained respectively for the PBC (Ferdinand and Fisher 1969) and for an infinite cylinder of width L (Onsager 1944).

The finite-size behaviour of the magnetic properties (χ and $|M|$) is not known analytically even for PBC, hence we compare our results to Fisher's finite-size scaling theory (Fisher 1970, Fisher and Barber 1972). According to this theory (Domb 1965, 1970, Gunton 1968, Watson 1972, Müller-Krumbhaar and Binder 1972) the susceptibility χ of a finite $L \times L$ lattice should increase with L as

$$\chi = BL^{\gamma/\nu} \qquad \text{at } K_c \text{ and for large } L \tag{11}$$

where B is a constant and γ and ν are the exponents related to the susceptibility and to the correlation length, respectively. A similar relation is expected for $|M|$, the exponent $-\beta$ replacing γ. A plot of $\log \chi$ against $\log L$ gave a straight line with slope 1.80 ± 0.12, while the expected theoretical value is 1.75. This is slightly better than 1.85 ± 0.08 obtained for γ by the SM method (MA). We also obtain $B = 0.45 \pm 0.1$, compared to $B = 0.7 \pm 0.1$ obtained by MA and $B = 1.00 \pm 0.04$ obtained with the Metropolis method (Landau 1976). The absolute magnetisation decreases with increasing L (except for $L = 120$) but the decrease is less than that corresponding to the expected value $\beta = \frac{1}{8}$. The above estimates for γ, based on the finite-size scaling theory, deviate 3–6% from the theoretical value and the range of error is relatively large. A new method, based on renormalisation group considerations, has been recently suggested (Swendsen 1979a, b, Blöte and Swendsen 1979) which enables one to estimate the exponents from computer simulation results at K_c. The method has been successfully applied to very long Monte Carlo runs at K_c for the square and cubic Ising lattices and for other plane models. It would be of interest to apply the Swendsen analysis to our results at K_c, where relatively small samples are required.

Let us now discuss some computational aspects of the present method and the SM method (MA). For $K \neq K_c$ we use here samples of 5000 configurations, compared to 1000 configurations used by MA. For several temperatures we also enlarge the lattice size from 90 to 120. This causes an increase in computer time which is necessary for accurate determination of the optimal parameters t^* and f^*; however, it enables us also to increase the accuracy of F significantly as previously discussed. A substantial saving in computer time is achieved with the present work, compared with the SM method (MA), by the fact that 2, rather than 10, parameters should be optimised. We decrease the computer time further by initially obtaining crude estimates of the optimal parameters from smaller samples, and then refining them by increasing the sample size.

The results obtained with the Metropolis method (besides $L = 76$ at K_c) are taken from MA. For each temperature they have been obtained from one Monte Carlo run, i.e. no attempt has been made to examine their accuracy, by carrying out more runs with different starting configurations and different random number sequences. For

$K \neq K_c$, 10^4 lotteries per spin (lps) gave generally good results, besides the too low values obtained for χ at $K = 0.40$, 0.43 and $K = 0.46$. This indicates that much larger samples are required. A detailed analysis, based on an approximate formula for the fluctuation in the magnetisation (Müller-Krumbhaar and Binder 1973) has been carried out by MA and led to the conclusion that for $K < K_c$ the sample size used should be increased by a factor of 2–10 in order to obtain accuracy of about 5% for χ. At $K = K_c$, however, where much stronger correlations exist between the sampled configurations the results obtained by MA for χ are exceedingly poor, which means that very large samples are required. In fact, huge samples have been used in Monte Carlo studies of the square Ising lattice, for example: samples of about 10^5 lps have been studied at $K = 0.425$ (Ogita *et al* 1969); at K_c Swendsen uses 9×10^4 lps for $L = 45$ (Swendsen 1979a) and 3×10^4 lps for $L = 108$ and $L = 81$ (Swendsen 1979b). From our experience this last sample is still insufficient for obtaining good estimates of χ. With the SM procedure, in contrast to the Metropolis procedure, the sampled configurations are statistically independent and therefore much smaller samples are required. On the other hand, one has to optimise the two parameters. In view of the results of the present method and the discussion of MA about the SM and the Metropolis methods we conclude that, as far as the square Ising lattice is concerned, the efficiency of the two methods is comparable for $K \neq K_c$; at K_c, however, the present method gives reasonable results for χ whereas the results obtained with the Metropolis method are exceedingly poor.

5. Conclusions

In this work we define the TP for the SM method in a novel way, which is based on rigorous considerations, and apply the method, as a test, to the square Ising lattice. The new method is found to be comparable in efficiency to the MC method and significantly more efficient than the SM method studied previously (Meirovitch and Alexandrowicz 1977a). Very high accuracy is obtained for the free energy $F(\sim 10^{-6}$, not too close to T_c), much better than obtained with the MC method (Meirovitch and Alexandrowicz 1977b) or with other approximations for the square Ising lattice (Burley 1972 and references therein). These results are important since from F one can derive all the thermodynamic quantities of a system. Also, the minimum free energy principle constitutes a criterion for defining the most stable state of a system, which is useful when different simulation runs lead the system to different free energy minima. F is also important in the case of a first-order phase transition, where two phases with the same free energy coexist. Near such transitions the MC method (because of long-range *time* correlations) gives rise to hysteresis loops (Landau and Binder 1978), which make it difficult to determine the transition point precisely. However, with the present method, which is not of a relaxation type, the hysteresis loops do not occur and one can construct the two phases and define the transition point accurately, by comparing their free energies (for details see Meirovitch 1977b). We expect, therefore, the present method to be more effective than the MC method for systems which undergo first-order transitions such as lattice gas models with nearest-neighbour exclusion and second (and third) neighbour interactions (Kinzel and Schick 1981), or Ising antiferromagnets in an external magnetic field (Binder and Landau 1980). The present method (as well as the MC method) can also be applied to problems which were not solved with sufficient accuracy by other methods. For example, the estimation of the

critical exponents α and γ for the hard-square lattice gas by series expansion is unsatisfactory (Baxter *et al* 1980). Applying Fisher's finite-size scaling theory (Fisher 1970, Fisher and Barber 1972) or Swendsen's method (Swendsen 1979a, b) to the simulation of this model with the present method might provide more accurate results. Finally, it should be pointed out that, in view of the poor convergence of the MC results, near phase transition, it is of interest also to have the present method (which is approximate but shows much faster convergence) as an alternative computer simulation technique.

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