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The Monte Carlo method and correlated boundary conditions

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Abstract. We have proposed new boundary conditions for use in Monte Carlo simulations and have applied them in this instance to the two-dimensional square Ising model. The variables defined on the first layer outside the boundary of the system are determined by the requirement that the nearest-neighbour pair correlation function, with the boundary spin as one of the pair, is equal to that calculated from the finite system. The single-site values of the variables outside the boundary are chosen with a probability consistent with the fluctuations in the pair correlation function for the finite system.

1. Introduction

The Monte Carlo method (MCM) is a powerful tool in the study of models of cooperative phenomena (Binder 1979). Essentially the MCM is a means of estimating a multi-dimensional integral, related to the thermodynamic quantities of interest, through the use of random numbers. The random numbers are used to generate a sample population (configurations) from which statistical estimates are obtained. An appraisal of the technique in general applications, i.e. in all areas, indicates that the MC estimate of an integral is a consistent estimate, i.e. it converges to the right answer as the sample size becomes very large (James 1980). When this method is used to study cooperative phenomena in equilibrium statistical mechanics, the accuracy is less. Thus a statement which until recent times (Heermann and Stauffer 1981) was not uncommon was 'Monte Carlo results are only accurate to within 10% when compared with exact values in critical phenomena'.

We briefly discuss some of the potential sources of difficulties. There are a number that can be identified immediately. (a) The problems of interest require taking the thermodynamic limit, i.e. $N \to \infty$ where N is a length defining each dimension of the system. In practice, of course, one is constrained to study systems of finite size from which one must deduce the properties of an infinite system. (b) We are particularly interested in the critical properties of the system and near the critical temperature the relaxation time of the order parameter is finite but large—the phenomenon referred to as critical slowing down. This means that the closer one gets to the critical point, the greater the required CPU time to achieve the desired sampling of independent states. (c) Boundary conditions, therefore, play an important role in the MC simulation of finite systems. Instead of divergence of the thermodynamic properties, periodic boundary conditions lead to 'rounding errors' and the thermodynamic properties are usually analysed through finite size scaling. In some instances the results for systems of various sizes are obtained and plotted against an inverse power of N and the values

relevant for the infinite system are deduced from an extrapolation to the limit $1/N \to 0$. It should be pointed out that periodic boundary conditions enhance fluctuations—the growth of droplets at an edge continues at the opposite side—thus leading to an overestimate of response functions in the critical region. A major drawback with these conditions is that the correlation functions are only reliable to order $N/2$ (half of the width of the system!). Another feature is that there is never a sharp transition; the order parameter remains non-zero for $T > T_c$. Müller-Krumbhaar and Binder (1972) proposed an alternative set of boundary conditions—an external field acts on the boundary spins with the condition $\partial m/\partial n = 0$ where n is a direction normal to the local boundary. This is a generalisation of the Bethe approximation and as such leads to a sharp transition, but a crossover to classical exponents is observed near the critical temperature. These boundary conditions should be appropriate for studying first-order phase transitions where there is usually an absence of critical fluctuations. (d) Most MCM use pseudo-random numbers. It has been shown that these are not truly random but fall on hyperplanes (Marsaglia 1968). This is a feature of all random number generators and the spacing between the planes is related to the length in bits of the computer word. It is difficult (if not impossible) to estimate the errors associated through the use of numbers which are not truly random.

Intuitively one might expect that the proper implementation of a MC study should yield results of the same order as the high temperature series expansion (HTSE), i.e. MCM results for a 40×40 lattice should be of the same order as, say, HTSE for graphs of up to order ~ 20. That this appears not to be true arises from the fact that HTSE to order $N/2$ give more accurate results than are obtained using MC techniques on $N \times N$ lattices. In § 2 we present the new boundary conditions which are designed to mimic the infinite system, whilst in § 3 a novel means of sampling in the critical region is introduced.

2. New boundary conditions

Can we calculate the properties of an infinitely large system arbitrarily accurately by observing the properties of a finite portion (sample) of this system for a sufficiently long time? The answer, at first sight, appears to be yes, because all of the sample's configurations with the correct frequencies will appear over an infinitely long period of observation. The use of boundary conditions proposed here is, thus, to fool the system into 'believing' that it is part of an infinitely large system. The boundary conditions which are generally used are single-site boundary conditions, i.e. they assign values to the variables of the first layer outside, either by calculating single-site averages inside (mean field conditions) or by making using of single-site values, e.g. cyclic boundary conditions. Instead of using single-site conditions to define the state of the spins in the first layer outside the finite system, we have made use of a method which determines these states through the use of the pair-correlation function and the average magnetisation. The state of each spin on the first layer outside the boundary is dependent on a random number which is compared with $x_{AA}(r)$ (the probability that the spin at distance r is up, given that the spin at the origin is up) or $x_{BB}(r)$, the converse.

These probabilities are related to the correlation function (Harding and Bunyan 1980). Consider the following projection operators at a given site:

$$A = \tfrac{1}{2}(1+S) \qquad B = \tfrac{1}{2}(-S) \qquad S = \pm 1 \tag{1}$$

where A is 1 for S up and 0 otherwise. The converse is true of B. The fractional compositions of up and down spins are

$$x_A = \tfrac{1}{2}(1 + \langle S \rangle) \qquad \text{and} \qquad x_B = \tfrac{1}{2}(1 - \langle S \rangle) \tag{2}$$

where $\langle S \rangle$ is the magnetisation of the system.

The probability that a spin at r is up, given that the one at the origin is up, is

$$x_{AA}(r) = x_A(x_A + x_B\Gamma(r)) \tag{3}$$

and similarly

$$x_{BB}(r) = x_B(x_B + x_A\Gamma(r)) \tag{4}$$

where

$$\Gamma(r) = (\langle S_0 S_r \rangle - \langle S_0 \rangle^2)/(1 - \langle S_0 \rangle^2). \tag{5}$$

Thus the first layer of spins outside the system is assigned a state such that this layer has approximately the same magnetisation as the system, but in addition we have built in the nearest-neighbour correlations between these spins and their internal neighbours. Thus we may look upon these boundary conditions as an improved mean field. However, the states of these spins are not fixed but are allowed to change with the same frequency as the spins of the interior of the system. These conditions are very close in spirit to the extended mean-field approximation of Bolton and Johnson (1976) and the self-consistent fluctuating mean field of Jan (1977). In the latter case the magnetisation of the external layer of spins is selected and adjusted to ensure that it has the identical distribution to the internal magnetisation of the sample, but at a given instant the internal magnetisation of the sample and the external layer magnetisation are not necessarily the same.

3. Sampling in the critical region

Near T_c the relaxation time of the order parameter is long and this has the effect that the MC program will sample only a small region of phase space in a given run. The averages calculated for the various thermodynamic properties obtained from such a set of configurations will not be statistically independent and, furthermore, will strongly depend on the initial configuration. In addition, there is need to simulate the effects of the external portion of the system. In the critical region there are fluctuations ranging from the microscopic level to the macroscopic size of the system. We attempt to take this behaviour into account through a temperature fluctuation in a portion of the sample; thus a region varying in size from a few spins to approximately the size of the largest cluster observed for that given temperature is selected at random and a droplet is created by flipping over these spins from their present state to the opposite state. The system is allowed to attain equilibrium and further 'typical' configurations are generated. The overall effect should result in the sampling of another region of phase space and thus for a given amount of computing time an independent set of configurations. Far from and below T_c the droplets are small and thus only a small cluster of spins will be perturbed, but after a few MC steps, this droplet disappears and there is no discernible difference between these equilibrium configurations and those obtained in the traditional manner. The same applies for the system above T_c. However, near to T_c the droplets are large and thus the perturbing of a portion of

the system is equivalent to a new initial configuration but one where there are some initial long range correlations.

4. Results

The relevant thermodynamic averages and fluctuations

$$\langle A\rangle = K^{-1}\sum_{i=1}^{K} A_i \tag{6}$$

$$\langle \Delta A^2\rangle = \langle (A-\langle A\rangle)^2\rangle \tag{7}$$

are calculated in the usual manner, where K is the number of MC steps. In particular, the magnetisation is

$$M = K^{-1}\sum_{i=1}^{K}\langle S\rangle_i \qquad M(T) = |M|. \tag{8}$$

The variation of the nearest-neighbour, next-nearest-neighbour and third-nearest-neighbour correlation functions with temperature is shown in figure 1 for the 32×32 lattice. There is a sharp fall in the values of these variables near the critical temperature of the finite system. Figure 2 shows the variation of the average energy

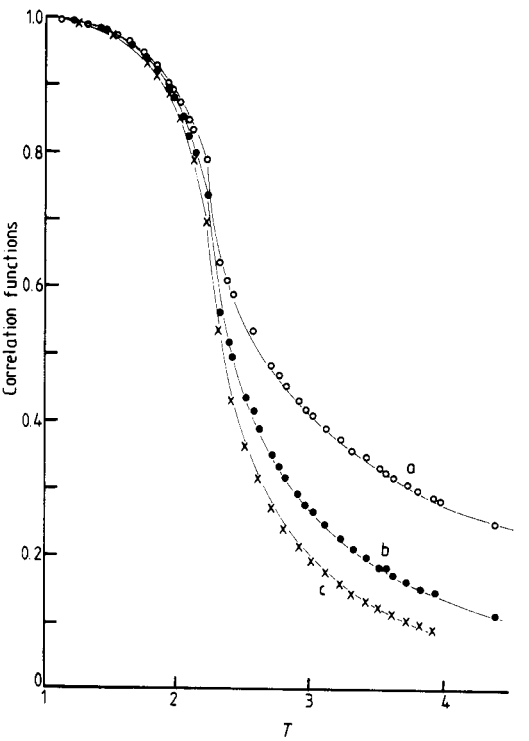

Figure 1. The correlation functions against temperature: a, nearest-neighbour, b, next-nearest-neighbour, c, third-nearest-neighbour. The full lines are the exact results of McCoy and Wu (1973).

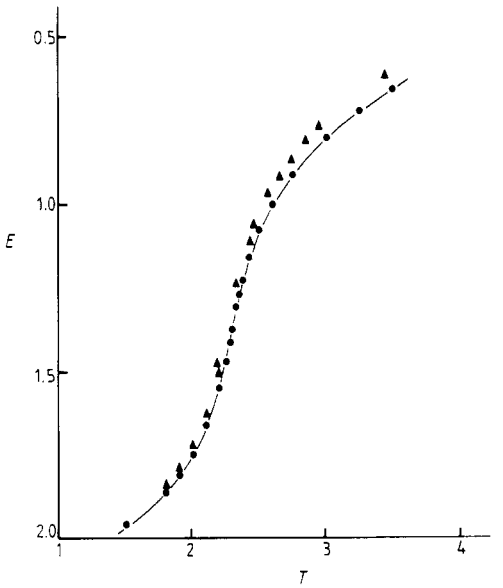

Figure 2. The energy E (●) against temperature. The full line is the exact result of Onsager (1944). ▲ are the values obtained with periodic boundary conditions.

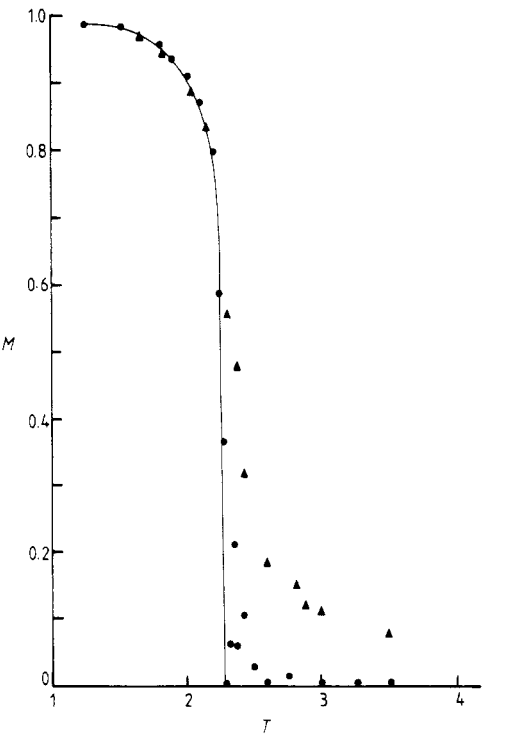

Figure 3. The spontaneous magnetisation M (●) against temperature. The full line is the exact result of Yang (1952). ▲ are the results obtained with periodic boundary conditions.

per spin with temperature. There is a noticeable change in the gradient of this curve near $T \sim T_c$ (exact). We have also simulated the properties of an 8×8 system with correlated boundary conditions and notice that the greatest discrepancy with the larger system occurs in the critical region.

The variation of the magnetisation with temperature (figure 3) shows remarkable agreement with the exact results for $T \leqslant 2.25$. Our results, however, indicate a critical temperature of 2.230 as compared with the exact value of 2.268. There are strong fluctuations in the magnetisation above T_c and it is only for the values of $T > 2.50$ that the absolute value of the magnetisation is aways less than 0.1. The specific heat and susceptibility (figures 4 and 5) also show the expected increases. The major source of error in the analysis of the critical exponents will be due to the error in the critical temperature.

5. Conclusion

The MC technique is a powerful means of simulating systems which exhibit phase transitions and critical phenomena. The two-dimensional Ising model presents the greatest challenge for computer simulations, mainly due to the slow decay of the long range correlation functions and the existence of exact values for comparison. We have presented a new set of boundary conditions which are designed to minimise the effects

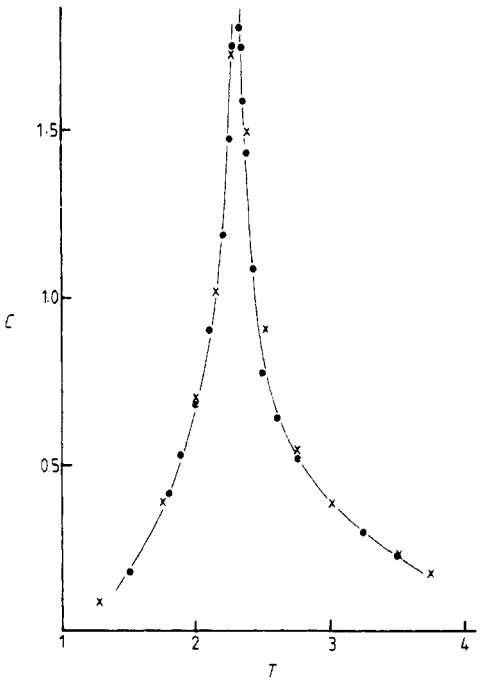

Figure 4. The specific heat C (●) of the two-dimensional Ising model as a function of temperature. The full line is the exact result of Onsager (1944). × are the exact values for a 32×32 lattice with periodic boundary conditions (Ferdinand and Fisher 1969).

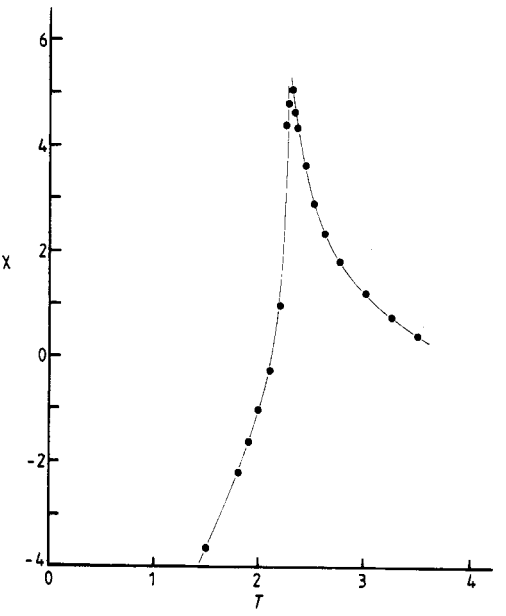

Figure 5. The susceptibility χ (●) as a function of temperature. The full line is a guide to the eye.

of the slow decay of the correlations near T_c and have tested our method on the 2D square Ising ferromagnet. The results are consistent, e.g. the magnetisation, specific heat and susceptibility all indicate the same critical temperature.

There remains, however, an outstanding problem with these (and most) boundary conditions—adequate sampling in the critical region. The relaxation time of the order parameter near T_c is very long and an additional element is needed to ensure that there is appropriate sampling of phase space in the critical region. This is not crucial with the use of periodic boundary conditions in small systems as these conditions encourage the artificial growth of droplets. We have made an initial effort to address this problem but a more systematic approach is required.

Finally, it should be noted that we have used a site-selection procedure intended to circumvent the possibility of getting locked into a region of phase space because of the order in which the sites have been visited. In our simulation sites were selected at random to be visited once and only once in each MC step, and the order in which they were visited varied with each step.

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