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Monte Carlo simulation of model spin systems*

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Abstract. In this paper, applications of the Monte Carlo technique to estimate the static and dynamic properties of model spin systems are discussed. Finite-size effects and choice of boundary conditions in simulating different types of real systems are outlined. Various applications of the Monte Carlo simulations to one-, two- and three-dimensional Ising models and Heisenberg models are dealt with in some detail. Recent applications of the Monte Carlo method to spin glass systems and to estimate renormalisation group critical exponents are reviewed.

Keywords. Monte-carlo simulation; critical phenomena; Ising models; Heisenberg models; spin glass; renormalisation group

1. Introduction

Model systems are helpful in understanding the static and dynamic aspects of critical phenomena. Unfortunately the model systems, excepting some one-dimensional models and two-dimensional Ising models, are not solvable exactly. This necessitates the use of approximate methods to deal with such systems. Often, such approximate methods used in solving the models lead to spurious results. However, by a Monte Carlo simulation, the approximations can be bypassed and the model can be studied directly to obtain useful static and dynamic properties of the system. This apart, the Monte Carlo method has the advantage of giving a good physical insight into the model, by providing the detailed microstructure of the system at any stage of the computation.

The drawbacks of a Monte Carlo simulation generally are the finite sample size and the finite system size. However, a finite system size has the advantage of allowing one to study finite size effects on the critical phenomena, an aspect which has been of much recent theoretical interest.

In § 2 of this paper we shall discuss the basis of the Monte Carlo method and its practical realisation. We shall also discuss methods of estimating static and dynamic properties of a given system. Detailed discussions of these aspects can be found in review articles by Binder (1974a, 1976). In § 3 we shall briefly review the results of the Monte Carlo calculations carried out on Ising models, classical Heisenberg models and spin glass models, in various dimensions. We shall also discuss recent applications of the Monte Carlo method for obtaining critical exponents *via* the renormalisation group approach.

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2. Monte Carlo method and thermodynamics of spin systems

2.1 *Static properties*

Equilibrium statistical mechanics is concerned with calculations of averages of the type

$$\langle F\rangle = \sum_{i}^{\text{over all states}} \exp(-\beta E_i) F_i \Big/ \sum_{i}^{\text{over all states}} \exp(-\beta E_i), \tag{1}$$

where E_i is the energy of the state i, F_i is the value of the variable in state i and $\beta = 1/k_B T$. This sum is reduced to an integration over configuration space for classical systems. We would, however, be concerned mostly with properties of the system which depend only on spatial co-ordinates. Hence, the above sum can be replaced by an integral of the form

$$\langle F\rangle = \int F(r) \exp[-\beta U(r)]\, dr \Big/ \int \exp[-\beta U(r)]\, dr, \tag{2}$$

where $U(r)$ is the potential energy of interaction among particles and r designates all the space variables of the system.

In this paper since we would mostly be dealing with discrete energy states, we shall use (1) for calculating expectation values. Equation (2) is used mostly in liquid state calculations and the like.

For an Ising system of N spins, a straightforward evaluation of equation (1) requires a summation over 2^N terms in the numerator and the denominator, corresponding to 2^N configurations in which the N spins can exist. This ' unmanageable ' problem can be overcome if we adopt a Monte Carlo method for estimating the sums. We cannot use a simple Monte Carlo sampling where the probability $P(i)$ for selecting any configuration i is 2^{-N}. Such a sampling will require enormous computation time since all the configurations are *not* equally probable at equilibrium. The probability for any configuration i at equilibrium is given by

$$P(i) = \exp(-\beta E_i) \Big/ \sum_{i}^{\text{over all states}} \exp(-\beta E_i). \tag{3}$$

A better sampling technique would be the ' importance ' sampling technique with the probability for a configuration given by (3). This requires an understanding of the denominator in (3). However, knowing the denominator is itself equivalent to solving the problem since the denominator is the partition function of the system. We set out to estimate thermodynamic properties by the Monte Carlo method since exact determination of the partition function was not possible and we did not want to solve the model by using any approximate method. It appeared as though we had ended up in a vicious circle. A way out of this was devised by Metropolis *et al* (1953). They devised a Markov chain for generating the configurations of the system. This Markov chain has all its states belonging to the same class i.e., any state of the Markov chain is attainable from any other state, and is also ergodic. The

limiting probabilitiy of this Markov chain is the same as the equilibrium probability of the system. Thus the Monte Carlo estimate of equilibrium thermodynamic properties involves the following steps.

(i) Generate the states of a Markov chain defined by judiciously chosen initial probability and one-step probabilities such that the Markov chain is ergodic and the ergodic probabilities for the states of the chain are the same as the equilibrium probabilities.
(ii) Allow the Markov chain to make a reasonable number of transitions so that the Markov chain has reached the limiting behaviour.
(iii) Average the desired property over a large number of configurations starting from the time it has reached a atisfactory limiting behaviour.

Thus the Monte Carlo estimate of a property F is

$$\langle F \rangle = \frac{1}{M} \sum_{i=N+1}^{N+M} F_i, \tag{4}$$

where N is the number of steps required to reach the ergodic limit and M is the number of configurations over which the property is averaged so as to obtain the desired accuracy. Discussion of error estimates due to choice of finite N and M is postponed to the next subsection as it requires understanding the dynamics of approach of the system to equilibrium and the time correlation of equilibrium fluctuations of the desired property.

For a Markov chain with states belonging to the same class to be ergodic, the one-step probabilities and the limiting probabilities should satisfy the following conditions:

$$\sum_{k}^{\text{over all states}} P_{kj}^{(1)} = 1, \quad \text{for all } j \tag{5a}$$

and

$$\pi_j P_{jk}^{(1)} = \pi_k P_{kj}^{(1)}, \tag{5b}$$

where $P_{kj}^{(1)}$ are the one-step probabilities for going from state k to state j and π_j is the limiting probability for the state j. Since π_j should be the equilibrium probability we have $\pi_j \propto \exp(-\beta E_j)$ where E_j is the energy of the configuration j. One way of satisfying the above conditions would be the following (Wood & Parker 1957):

$$\begin{aligned} P_{jk}^{(1)} &= A_{jk} \text{ for } E_j \leqslant E_k, \\ P_{jk}^{(1)} &= A_{jk} \exp\left[-(E_j - E_k)\beta\right] \text{ for } E_j > E_k, \\ P_{jj}^{(1)} &= 1 - \sum_{k \neq j} P_{jk}^{(1)}. \end{aligned} \tag{6}$$

The initial probability $P_i^{(0)}$ of the chain is chosen such that $P_i^{(0)}$ is 1 for some specific state i and zero for all the rest, or, $P_i^{(0)}$ is 2^{-N} for all the 2^N configurations of the chain.

In this paper we will concentrate on two types of spin systems viz., the spin-half Ising systems and the classical Heisenberg systems.

The spin-half Ising system is described by spins arranged either up ($S^z = +\frac{1}{2}$) or down ($S^z = -\frac{1}{2}$) at lattice points and interacting via a Hamiltonian of the form

$$H = \sum_{i>j} J_{ij}\, S_i^z\, S_j^z - H^{\text{ext}} \sum_i S_i^z, \tag{7}$$

where J_{ij} is the exchange interaction between the spins at sites i and j and H^{ext} is the applied field. The practical realisation of the Monte Carlo averaging of thermodynamic properties of an Ising chain involves, firstly, generation of the system on a computer in the given (ordered or disordered) initial state. The sequence of configurations of the system are then generated by locating a site at random and calculating the probability for flipping the spin at that site using (6) and (7). This probability is compared with a random number generated between 0 and 1. If the calculated probability is larger than the random number, the spin at the site is flipped to obtain a new configuration. Otherwise the earlier configuration itself is considered as the new configuration. This mechanism of generating the states of the Markov chain is known as the single spin-flip mechanism and has been found to be very efficient in general. After a reasonable number of steps we begin computing the desired thermodynamic properties of each generated configuration and at the end of the computation the averages of these properties are calculated and taken as the Monte Carlo estimates (equation (4)).

The Hamiltonian of a classical Heisenberg model in an external field is given by

$$H = \sum_{i>j} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j - H^{\text{ext}} \sum_i S_i^Z, \tag{8}$$

where $\mathbf{S}_i$ and $\mathbf{S}_j$ are unit vectors at sites i and j. J_{ij} is the strength of exchange interaction and H^{ext}, the applied field. Monte Carlo realisation of this model involves starting from a random or fixed orientation of unit vectors at the lattice sites depending upon whether the initial state is a random or an ordered state. Different states of the Markov chain are then generated by choosing a site at random and selecting a new orientation of the spin at that site randomly using three random numbers ξ_x, ξ_y and ξ_z between 0 and 1 such that the components of the new orientation are given by

$$(S_i^z)' = (S_i^z + \xi_z \Delta)\,/\,Z,\ (S_i^x)' = (S_i^x + \xi_x \Delta)\,/\,Z,$$

$$(S_i^y)' = (S_i^y + \xi_y \Delta)\,/\,Z,\ Z = [(S_i^x)'^2 + (S_i^y)'^2 + (S_i^z)'^2]^{1/2}, \tag{9}$$

where S_i^x, S_i^y and S_i^z are the components of the old orientation and Δ is a parameter chosen so as to improve convergence. This new orientation is accepted with a probability calculated from (6) and (8). By repeating this procedure the Markov chain sequence is generated and as in the Ising case the estimates of various thermodynamic properties of the Heisenberg model are carried out.

The static properties that are generally computed are the total energy $\langle E \rangle$, the net magnetisation $\langle M \rangle$, given by

$$\langle M \rangle = \langle \sum_i S_i^z \rangle, \tag{10}$$

and the spatial correlation function $g(n)$, given by

$$g(n) = \langle \sum_i S_i^z \; S_{i+n}^z \rangle . \tag{11}$$

These are calculated for various values of the parameters of the model, as a function of temperature. The specific heat of the system can be estimated as the slope of the $\langle E \rangle$ vs T plot, and similarly, magnetic susceptibility, as the slope of $\langle M \rangle$ vs H^{ext} plot at $H^{\text{ext}} = 0$. One can also estimate the specific heats and magnetic susceptibilities from fluctuations in internal energy and the magnetisation respectively. The relations are

$$C_v \propto \frac{1}{T^2} (\langle E^2 \rangle - \langle E \rangle^2), \tag{12}$$

and

$$\chi \propto \frac{1}{T} (\langle M^2 \rangle - \langle M \rangle^2), \; \propto \frac{1}{T} \sum_n g(n). \tag{13}$$

The studies on model spin systems are carried out mainly to understand the phase transitions exhibited by these systems. The phase transitions of the second order are generally characterised by a set of exponents known as the critical exponents and these critical exponents describe the variations of thermodynamic properties near the phase transition. Some common critical exponents that one comes across in the study of phase transitions are α, α', β, γ, γ', δ, ν and η. These are defined by the relations

$$\begin{aligned} C &\sim (-\epsilon)^{-\alpha'} && \epsilon < 0, \\ C &\sim (\epsilon)^{-\alpha} && \epsilon > 0, \end{aligned} \tag{14}$$

$$M \sim (-\epsilon)^{\beta} \qquad \epsilon < 0, \tag{15}$$

$$\begin{aligned} \chi &\sim (-\epsilon)^{-\gamma'} && \epsilon < 0, \\ &\sim (\epsilon)^{-\gamma} && \epsilon > 0, \end{aligned} \tag{16}$$

$$H^{\text{ext}} \sim M^{\delta} \qquad \epsilon = 0, \tag{17}$$

$$\begin{aligned} \xi &\sim (-\epsilon)^{-\nu'} && \epsilon < 0, \\ &\sim (\epsilon)^{-\nu} && \epsilon > 0, \end{aligned} \tag{18}$$

$$g(r) \sim |r|^{-(d-2+\eta)} \quad \epsilon = 0. \tag{19}$$

Here, ξ is the correlation length, d is the dimensionality and ϵ is the temperature variable defined by

$$\epsilon = (T - T_c)/T_c, \tag{20}$$

where T_c is the critical temperature. All these relations are defined in the neighbourhood of T_c, whenever the defining relation assumes a non-zero ϵ.

One of the major aims of the Monte Carlo method in the study of model spin systems is to accurately estimate these critical exponents. We shall come back to a discussion of these aspects in § 3.

2.2 *Dynamic properties*

The dynamical interpretation of the Monte Carlo method is based on the concept that with each Monte Carlo step one can associate a time scale τ such that when the chain has gone through N Monte Carlo steps, we can say that the chain has evolved over a time $N\tau$. From the probability prescription we have used in the previous subsection we can see that the evolution of the chain is governed by the master equation*,

$$\frac{d}{dt}P(S_1^z, \ldots, S_i^z, \ldots, S_N^z, t) = -\sum_{i=1}^{N} W(S_i^z \to -S_i^z) \times P(S_1^z \ldots, S_i^z, \ldots, S_N^z, t) + \sum_{i=1}^{N} W(-S_i^z \to S_i^z) \times P(S_1^z, \ldots, -S_i^z, \ldots, S_N^z, t), \tag{21}$$

where $P(S_1^z, \ldots, S_i^z, \ldots, S_N^z, t)$ is the probability that the system is in the state $(S_1^z, \ldots, S_i^z, \ldots, S_N^z)$ at time t and $W(S_i^z \to -S_i^z)$ is the single spin-flip probability per unit time for flipping the ith spin. Since the Markov chain chosen for our study is ergodic, the probabilities satisfy the detailed balance condition of (5b). With this condition the master equation (21) becomes equivalent to the master equation of the single spin-flip kinetic Ising model proposed by Glauber (1963). Glauber's kinetic Ising model has been solved exactly in one-dimension and only approximately in higher dimensions. Thus Monte Carlo simulation provides a way of estimating time-dependent properties of the system without recourse to the approximate methods. The dynamic properties of interest in the study of phase transitions are the following.

(i) The time-dependent correlation functions, $\phi_{\delta A \delta B}(t)$, estimated as

$$\phi_{\delta A \delta B}(t) = \frac{N}{k_B T \chi_{\delta A \delta B}} \frac{1}{t_m - t - t_n} \int_{t_n}^{t_m - t} dt' [A(t') - \langle A \rangle] [B(t'+t) - \langle B \rangle], \tag{22}$$

where $\chi_{\delta A \delta B}$ is proportional to $1/T \times [\langle AB \rangle - \langle A \rangle$ and $\langle B \rangle]$ and t_n corresponds to the time when the Markov chain has reached the limiting behaviour. The upper limit of the integration is based on the desired accuracy.

(ii) The autocorrelation functions, $\phi^A_{\delta A \delta B}(t)$, estimated as

$$\phi^A_{\delta A \delta B}(t) = \frac{t_m - t}{t_m - t - t_n} \times \frac{\sum_{i=1}^{N} \int_{t_n}^{t_m - t} [A_i(t) - \langle A \rangle] [B_i(t'+t) - \langle B \rangle] dt'}{\sum_{i=1}^{N} \int_{t_n}^{t_m} [A_i(t') - \langle A \rangle] [B_i(t') - \langle B \rangle] dt'}. \tag{23}$$

*For the sake of simplicity we shall henceforth consider the dynamics of the Ising models only.

Computations are carried out generally for A and B representing magnetisation and magnetisation, internal energy and internal energy or magnetisation and internal energy.

Associated with these correlation functions are the relaxation times

$$\tau_{\delta A \delta B} = \int_0^{t_m - t_n} \phi_{\delta A \delta B}(t)\, dt, \tag{24}$$

and

$$\tau^A_{\delta A \delta B} = \int_0^{t_m - t_n} \phi^A_{\delta A \delta B}(t)\, dt. \tag{25}$$

The variation of the quantities $\tau_{\delta A \delta B}$ and $\tau^A_{\delta A \delta B}$ with temperature, near the critical point T_c are governed by exponent relations of the type

$$\tau_{\delta A \delta B} \sim (-\epsilon)^{-\Delta'_{\delta A \delta B}} \text{ for } T < T_c,$$

$$\sim (\epsilon)^{-\Delta_{\delta A \delta B}} \text{ for } T > T_c, \tag{26}$$

and

$$\tau^A_{\delta A \delta B} \sim (-\epsilon)^{(\Delta^A_{\delta A \delta B})'}, \; T < T_c, \tag{27}$$

$$\sim (\epsilon)^{(\Delta^A_{\delta A \delta B})}, \; T > T_c.$$

As in the case of static properties, dynamic properties are estimated by the Monte Carlo method to arrive at the dynamic critical exponents.

So far, we were concerned with the equilibrium relaxation functions. We can also study by using the Monte Carlo method the approach to equilibrium by estimating the non-equilibrium relaxation functions, defined by the relation

$$\phi^{\Delta T, \Delta H}_{\delta A} = \frac{\langle A(t) - A(\infty) \rangle}{\langle A(0) - A(\infty) \rangle}. \tag{28}$$

The non-equilibrium relaxation function ϕ describes the approach of the system to equilibrium, if at $t = 0$, the temperature and the magnetic field were changed from T to $T + \Delta T$ and H to $H + \Delta H$ respectively. The associated relaxation times and critical exponent are designated respectively by

$$\tau^{\Delta T, \Delta H}_{\delta A}, \quad \Delta^{\Delta T, \Delta H}_{\delta A}.$$

The estimation of equilibrium and non-equilibrium relaxation times are also important in estimating the error involved in Monte Carlo calculations. The error in Monte Carlo calculations stems from two sources—(i) insufficient number of Monte Carlo steps excluded (from averaging) to get rid of the effect of initial configuration and (ii) statistical error in estimates because of the finite sample size. Müller-Krumbhaar & Binder (1973) showed that the number of Monte Carlo steps/spin

Δn that should be excluded from the averaging, in order to eliminate the effects of initial configuration, should satisfy the inequality

$$\Delta n >> \tau_{\Delta A}^{\Delta H,\ \Delta T}. \tag{29}$$

They further showed that error in estimates due to finite sample-size n is given by

$$(\delta\bar{A})^2 \approx \frac{1}{nN}\,[\langle A^2\rangle - \langle A\rangle^2]\,(1+2\tau_{\delta A \delta A}),\ \text{for}\ n >> \tau_{\delta A \delta A}. \tag{30}$$

N is the system size (number of spins considered). Since $\tau_{\delta A}^{\Delta H,\ \Delta T}$, $\tau_{\delta A \delta A}$ and $[\langle A^2\rangle - \langle A\rangle^2]$ all show critical divergence, near a critical point, the number of Monte Carlo steps Δn to be excluded becomes prohibitively large as also the sample-size n for a given $(\delta\bar{A})^2$. Thus it is not possible to estimate the thermodynamic properties, with any accuracy, arbitrarily close to the critical point by the Monte Carlo method. Hence studies only as close to T_c as $T_c \pm 0{\cdot}02\ T_c$ have been carried out employing the Monte Carlo method.

2.3 *Boundary conditions and finite size effects*

In the practical realisation of the Monte Carlo method, we are constrained to deal with systems of finite sizes i.e., systems with a finite number of spins. Consequently, the surface of the system gains importance, unlike in the experimental study of bulk behaviour. Apart from the surface, the finite-size behaviour of the system itself leads to important consequences. While surface effects can be eliminated by judicious choice of boundary conditions, finite-size effects cannot be eliminated in our simulations.

The commonly used boundary conditions in the Monte Carlo simulations are (i) free boundary conditions (ii) periodic boundary conditions (iii) anti-periodic boundary conditions and (iv) self-consistent effective field condition. In the free boundary condition,

$$\mathbf{S}\,(h, k, l) = 0, \tag{31}$$

for h, k, l lying outside the system. Thus this boundary condition treats the surface as a free surface. In the periodic boundary condition

$$\begin{aligned}\mathbf{S}\,(h, k, l) &= \mathbf{S}\,(h \pm n_1, k, l),\\ &= \mathbf{S}\,(h, k \pm n_2, l),\\ &= \mathbf{S}\,(h, k, l \pm n_3),\end{aligned} \tag{32}$$

where n_1, n_2 and n_3 are the system dimensions of a cubic lattice. This boundary condition eliminates the surface effects while the finite-size effects still persist. The

antiperiodic boundary conditions are used to study interfaces of two domains with opposite magnetisation. Thus,

$$\begin{aligned} \mathrm{S}(h, k, l) &= \mathrm{S}(h \pm n_1, k, l), \\ &= -\mathrm{S}(h, k \pm n_2, l), \\ &= -\mathrm{S}(h, k, l \pm n_3), \end{aligned} \tag{33}$$

simulates an interface on the YZ plane. Similarly we can simulate thin films using free boundary condition in one direction and periodic boundary condition in the other two directions. Using free boundary condition and different shapes for the system we can study rough surfaces.

The self-consistent effective field condition (Müller-Krumbhaar & Binder 1972) is not really a boundary condition but it provides a method of treating surfaces. In this method, the Hamiltonian of the infinite system is approximated by the Hamiltonian of a finite system and an effective field acting on the surface. The effective field on the surface is adjusted self-consistently so as to have the magnetisation in the bulk and the surface the same. This method leads to quicker convergence of the finite-size properties to the infinite-size values than the other boundary conditions.

Thermodynamic behaviour of finite-size systems has been discussed by Fisher & Barber (1972) in terms of the critical exponents of the corresponding infinite system. This finite-size scaling theory predicts that the shift in T_c of a finite-size system is governed by an exponent through the relation

$$T_c = \left[1 - \frac{T_c(N)}{T_c(\infty)}\right] aN^{-\lambda} \text{ as } N \to \infty; \tag{34}$$

λ was shown to be equal to $1/\nu$ (equation (18)) by Fisher. Similar relations for the behaviour of magnetisation, susceptibility, specific heat etc., near T_c, of finite systems with and without surface, have been predicted by the finite-size scaling theory. Some of these predictions are confirmed by Monte Carlo simulation of finite systems of different sizes, with and without free surfaces.

3. Applications to model spin systems

3.1 *Ising Models*

Monte Carlo simulation has been extensively employed to understand the static and dynamic behaviour of Ising models. Studies have been carried out on one-, two- and three-dimensional Ising models. In two- and three-dimensions studies have been carried out on different types of lattices. We shall deal with these studies starting from the one-dimensional Ising model.

3.1a *One-dimensional Ising models*

It is known that one-dimensional Ising models with only short-range interactions do not exhibit any critical behaviour. However, when the interaction between spins is of infinite-range and Kac form *viz.*

$$J_{ij} = a\gamma \exp(-\gamma \mid i-j \mid), \gamma \to 0, \tag{35}$$

the chain exhibits a phase transition. Ising chains with competing short-range and infinite-range interactions have been studied by Nagle (1970) and Theumann & Hφye (1971). Particularly interesting is the Theumann-Hφye Ising chain, which exhibits several first-order phase transitions in the ground state. The Hamiltonian of Theumann-Hφye Ising chain is given by

$$H = -J \sum_i S_i^z S_{i+1}^z - K \sum_i S_i^z S_{i+2}^z - \sum_{i>j} \phi(i-j)\, S_i^z S_j^z,$$

$$J < 0, K < 0, \tag{36}$$

and $$\phi(i-j) = a\gamma \exp(-\gamma \mid i-j \mid), a > 0, \gamma \to 0. \tag{37}$$

In the limit $\gamma \to 0$, the last term in (36) can be replaced by an equivalent neighbour interaction term *viz.*

$$a \times \sum_{i \neq j} S_i^z S_j^z.$$

The T=0 phase diagram of this system is shown in figure 1. The present author has carried out a Monte Carlo simulation of this Ising chain to understand the finite-

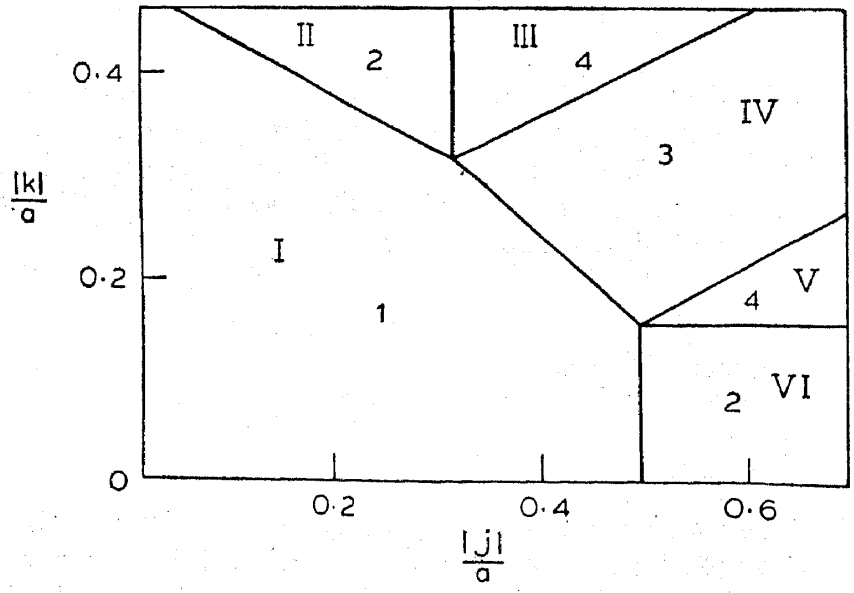

Figure 1. Phase diagram of Theumann and Hφye. j, k and a refer to the nearest neighbour, next nearest neighbour and infinite-range interaction strengths respectively. Roman numerals define the division of the diagram into regions. Arabic numbers give the number of phase transitions in the respective region at 0, K.

temperature critical behaviour (Ramasesha 1977). Several phase transitions have been observed, the number depending on the region of the phase diagram, as a function of temperature. These phase transitions are generally of a higher order, except in region I (where the transition is first order and is accompanied by a change in short-range order), and are characterised by a change in long-range ordering of the spins from one type of sublattice spin structure to another. For instance in region II, the long-range order of chain changes from a four sublattice spin structure ($\uparrow\uparrow\downarrow\downarrow$) to a three sublattice spin structure ($\uparrow\uparrow\downarrow$) at the first transition and at the second transition the chain becomes a paramagnet. The asymptotic correlation functions indicating this behaviour are shown in figure 2.

Glauber's kinetic Ising model (§ 2.2) is exactly solvable in one-dimension. Thus in one-dimension, Glauber's model provides a true testing ground for the Monte Carlo estimates of dynamical properties. Figure 3 shows time-dependence of various time-dependent pair correlation functions calculated exactly and estimated from Monte Carlo method (Stoll *et al* 1973). The agreement is excellent and thus one can have reliable estimates of dynamical properties by employing the Monte Carlo method.

3.1b *Two-dimensional Ising models*

The partition function of a two-dimensional square Ising model was exactly

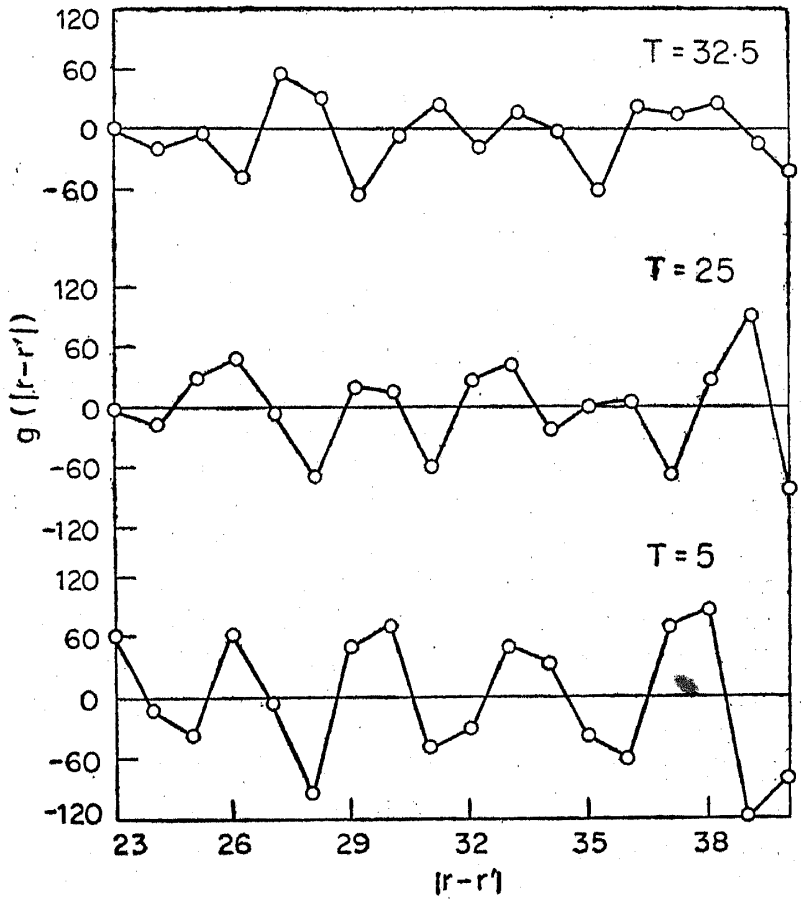

Figure 2. Plots of correlation functions vs distance, starting from the 23rd neighbour, for region II in zero field at different temperatures.

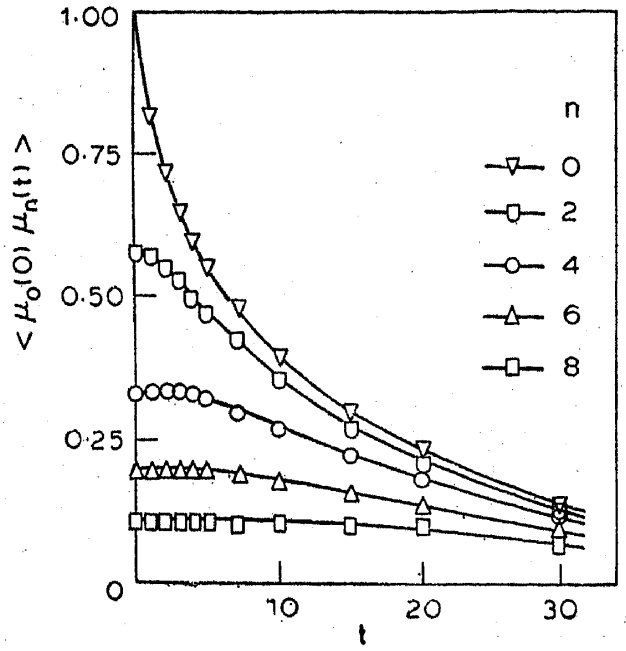

Figure 3. Calculated time-dependence of various pair correlation functions at $k_BT/J=1$ in the one-dimensional kinetic Ising model ($N=220$) with nearest neighbour interactions and periodic boundary conditions compared with exact results. After Binder (1976).

calculated by Onsager (1944) and he showed that the model exhibits a second-order phase transition. Since this is an exact result, most of the Monte Carlo calculations on two-dimensional square Ising models are carried out to check the accuracy of the calculations. We shall confine ourselves in the rest of this subsection to a square Ising lattice although there has been some recent work on order in a triangular Ising lattice (Meijer & Cunningham 1977).

Figures 4 and 5 give the variation of specific heat and magnetisation, with temperature for a 55×55 square lattice computed by Stoll *et al* (1973) and Binder (1974a, b). Also given for comparison are the exact results of Onsager (1944). We see from the figures that the fit with the exact results is excellent, for $|(T-T_c)/T_c|>0{\cdot}03$. Susceptibility and correlation lengths also agree very well with the exact results. As mentioned in the previous section, close to the critical point, the errors in the Monte Carlo estimates diverge. In two-dimensional Ising models, $(\gamma+\Delta_{\delta M\,\delta M})$ is much larger than in three dimensions and hence the error should be far more critical in two dimensions than in three dimensions. The good fit observed with the exact results, in spite of this drawback, shows the power of the Monte Carlo technique.

Several predictions about Fisher's droplet model, finite-size effects, site-dilute Ising models etc., have been tested in the case of two-dimensional Ising models through Monte Carlo estimates.

Fisher (1967) proposed the droplet model as a semi-phenomenological description of critical phenomena in Ising spin systems. According to this model, the free energy per spin is given by

$$F = -\mu_B H^{\text{ext}} - U_0 - k_B T \sum_{l=1}^{\infty} n_l, \qquad (38)$$

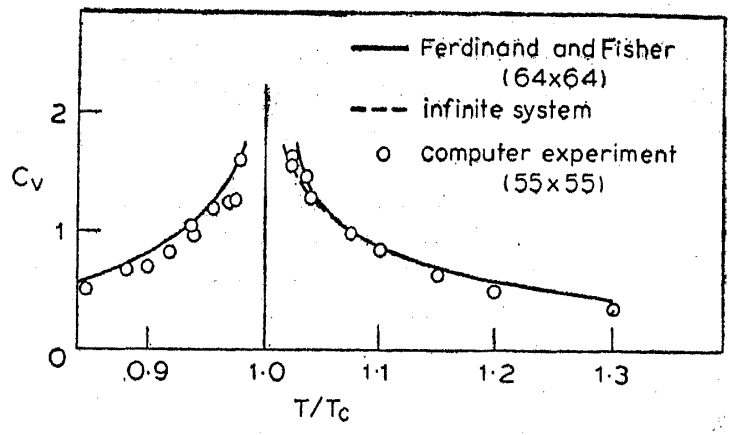

Figure 4. Specific heat of the Ising square 55×55 lattice, plotted vs reduced temperature. Full curve is the result of Ferdinand & Fisher for a 64×64 system, the dashed curve is the result of Onsager for an infinite system, and open circles are computer results of Stoll. After Binder (1976).

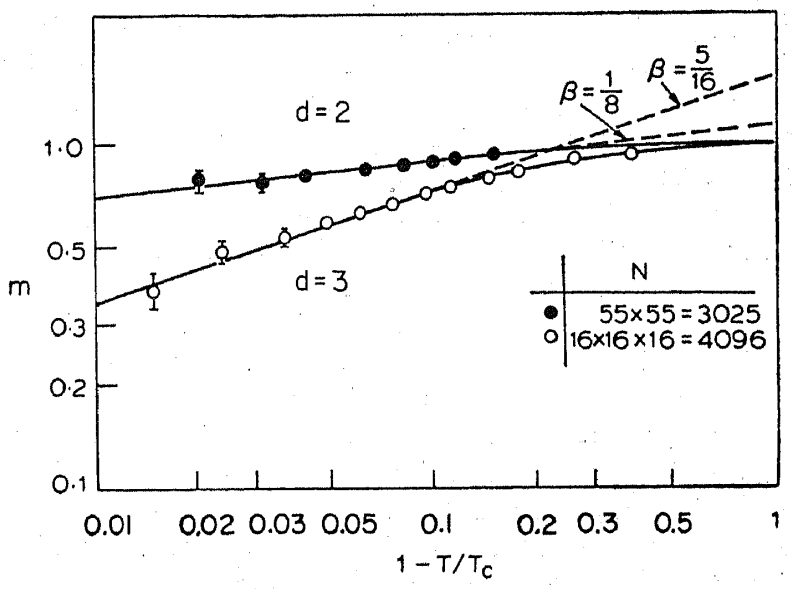

Figure 5. Log-log plot of the magnetisation of Ising lattice vs relative temperature $1\text{-}T/T_c$. Crosses denote Monte Carlo results of a square (d=2) lattices and open circles the Monte Carlo results of a simple cubic (d=3) lattice. The broken straight line is the result of Padé approximations. After Binder (1976).

where H^{ext} is the applied field, U_0 is the interaction energy in a fully aligned state and n_l is the cluster distribution function which gives the distribution of clusters with l reversed spins and has the form

$$n_l = q_0 \exp\left\{-\left[a_0 \frac{(T-T_c)}{T_c} \cdot \frac{J}{K_B T} l^{\sigma} + \frac{2\mu_B H}{K_B T} - 1\right]\right\} l^{-\tau}. \tag{39}$$

The constants q_0 and a_0 are related to the critical amplitudes and σ and τ are related to the associate critical exponents β and δ (15) and (17). In the two-dimensional Ising case Fisher proposed that σ has a value $\sim 3/5$ and $\tau \sim 31/15$. A Monte Carlo simulation study was carried out by Stoll *et al* (1972) to test the droplet model. They defined a cluster as a group of reversed spins linked together by at least one nearest

neighbour bond. The distribution function n_l calculated from this study was fitted to (39) assuming a value of 3/5 for σ. This gave a Monte Carlo estimate for the value of τ as $2{\cdot}1 \pm 0{\cdot}1$, in very good agreement with the value predicted by Fisher. Thus the droplet model seems to be a good description of the critical phenomena, at least in two dimensions.

Finite-size effects have been studied in two-dimensional Ising models, by Landau (1976), employing Monte Carlo method. He confirmed the predictions of the scaling theory of finite-size effects from the critical exponents for magnetisation, susceptibility and specific heats of finite systems. However, in the two-dimensional Ising case, it could not be ascertained if λ (equation (34)) generally has the non-scaling value of unity or has a value ν^{-1} (equation (18)) as the value of ν is unity in the two-dimensional Ising case.

Critical properties of site-dilute two-dimensional Ising models have also been studied by Ching & Huber (1976), employing Monte Carlo method. The studies are carried out for $p = 0{\cdot}7, 0{\cdot}8, 0{\cdot}9$, and $1{\cdot}0$ (p is the fraction of magnetic ions) on the square Ising lattice. The thermodynamic properties are averaged over five independent distributions of magnetic and non-magnetic ions for each concentration p. The plot of $T_c(p)/T_c$ (1) vs p was a straight line with a slight spread of the point for $p=0{\cdot}7$. The initial slope of the curve has a value of $1{\cdot}47 \pm 0{\cdot}05$, concordant with the series value of $1{\cdot}45 \pm 0{\cdot}05$. However, critical exponents do not seem to vary with p, in contrast to the results of series expansion.

Glauber's single spin-flip kinetic Ising model has been studied by the Monte Carlo method, on a square lattice by Stoll *et al* (1973), as well as by Bolton & Johnson (1976). Stoll *et al* computed the relaxation times $\tau_{\delta M \delta M}$, $\tau^{A}_{\delta M \delta M}$, $\tau_{\delta E \delta E}$, $\tau^{A}_{\delta E \delta E}$, $\tau_{\delta M \delta E}$ and $\tau^{A}_{\delta M \delta E}$. They found that the associated critical exponents satisfy the rigorous inequalities and lower bounds, computed by approximate methods. The exponent values are $\Delta_{\delta M \delta M} \approx \Delta_{\delta E \delta E} \approx \Delta_{\delta M \delta E} \approx 1{\cdot}90 \pm 0{\cdot}10$, $\Delta^{A}_{\delta M \delta M} \approx 1{\cdot}60 \pm 0{\cdot}10$, $\Delta^{A}_{\delta M \delta E} \approx 0{\cdot}95 \pm 0{\cdot}10$ and $\Delta^{A}_{\delta E \delta E} \approx 0$. These results are consistent with the predictions of the dynamic scaling hypothesis of Halperin & Hohenberg (1967, 1969). The results of Bolton & Johnson are based on a different boundary condition. However, their results also agree with the predictions of the dynamic scaling hypothesis.

Studies of metastable states and non-equilibrium relaxations have also been carried out on a square Ising lattice (Binder & Stoll 1973). In these calculations, the external magnetic field is suddenly reversed and the evolution of the system after reversal is followed. It is seen for some values of the reversed field that the non-equilibrium relaxation time, exceeds the order parameter relaxation times by several orders of magnitude. Such non-equilibrium states, which are also observed in real experiments are defined as metastable states. The critical exponent for the non-equilibrium relaxation conforms to the prediction of dynamic scaling hypothesis.

3.1c *Three-dimensional Ising models*

Systematic study of the three-dimensional Ising lattices (simple cubic and body-centred cubic) was carried out by Fosdick (1959, 1963) and Ehrman *et al* (1960). These workers computed the order-parameters and found excellent agreement with series extrapolation estimation. However, information about thermodynamic properties, such as specific heat and susceptibility is lacking in this case.

Finite-size effects have been studied by the Monte Carlo method in the case of a simple cubic lattice and the scaling law (34) has been confirmed. This was not possible in the two-dimensional case since the critical exponent was unity. The above study was carried out using both free and periodic boundary condition. It was found that with periodic boundary condition the effect of finite-size is small and that the asymptotic behaviour (34) is reached for small system size. Thus the 'rounding' effects observed in phase transitions of finite systems have been attributed to the free surface since with free boundary condition the asymptotic limit is reached only for much larger sizes of the system.

3.2 *Heisenberg models*

3.2a *One-dimensional Heisenberg model*

One-dimensional Heisenberg model does not show any phase transition. However, there are certain real systems whose behaviour closely approximates that of one-dimensional Heisenberg antiferromagnet which has not yet been solved exactly. One such system is tetramethylammonium manganese chloride (TMMC). To fit the experimental scattering function data available on TMMC, Windsor & Locke-Wheaton (1976) carried out a Monte Carlo calculation and estimated the spin correlation function $\langle S^*_{-q}(0)\, S_q(t)\rangle$. Scattering function calculated from this data is in remarkably good agreement with the experimental scattering function. The spin wave dispersion curves obtained from the Monte Carlo data show appreciable nonlinearity even at low temperatures.

3.2b *Two-dimensional Heisenberg model*

The two-dimensional Heisenberg model also does not exhibit any phase transition (Mermin & Wagner 1966). However, it was conjectured by Stanley & Kaplan (1966), that a special ordered state with 'long-ranged short-range order' exists in the two-dimensional Heisenberg model. The Monte Carlo simulation of Watson *et al* (1970) indeed failed to show any critical behaviour. But the short-range order was found to have a range as large or at times larger than the system dimensions.

3.2c *Three-dimensional Heisenberg model*

While extensive Monte Carlo calculations have been carried out on simple cubic lattices (Binder & Rauch 1969; Watson *et al* 1969), only a few calculations are available in the case of the body-centered cubic lattice (Binder *et al* 1970) and the face-centred cubic lattice (Paauw *et al* 1975). In the case of the simple cubic lattice the Monte Carlo estimates of β, γ, δ, ν and ν' ((15) and (18)) are found to be in very good agreement with the values predicted by series expansion methods. Simple cubic lattices with nearest and next nearest neighbour interactions have also been studied (Binder 1976) and the Monte Carlo estimates are found to agree very well with the series expansion calculations, wherever the latter has been performed. The three-dimensional Heisenberg model has also been studied using the self-consistent Monte Carlo method (Müller-Krumbhaar & Binder 1972) and the agreement with the

critical behaviour studied by series expansion methods was found to be quite satisfactory. Müller-Krumbhaar & Müller (1974) estimated the local order parameters of the three-dimensional Heisenberg model near the critical point. They calculated the distribution functions for magnetisation *viz.*, $p(M_1)$—of a single spin, $p(M_2)$—of a pair of neighbouring spins, $p(M_3)$—of three collinears pins and $p(M_7)$—of a central spin and its six neighbours. They found that the width of the distribution $p(M_1)$ showed a cusp-like behaviour, near T_c, in each case. This was used in interpreting some of the magnetic resonance results obtained on such systems.

3.3 *Spin glass models*

3.3a *Experimental and theoretical situation*

Spin glasses have been reviewed recently by Fisher (1977). They are dilute magnetic alloys formed by dissolving magnetic impurities in a non-magnetic host metal (e.g. *Au* Fe), and are characterised by a cusp in magnetic susceptibility at low temperatures and a broad maxima in specific heat at a temperature T_m roughly 20% higher than the cusp temperature T_f. In these systems, although Mössbauer lines are split due to a hyperfine field, no long-range order has been found below T_f. These systems also show strongly asymmetric hysteresis loops when cooled below T_f in an applied field. The remanence is found to decrease logarithmically with time. The temperature T_f varies as C^m, where C is the concentration of the magnetic impurity and m ranges between 0·55 and 0·75.

Spin glass property has been attributed, at a microscopic level, to the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction between magnetic moments which are randomly distributed. The RKKY interaction is long-ranged and oscillatory in behaviour. In spin glass theories, the RKKY interaction between the randomly distributed magnetic impurities is replaced by a randomly varying exchange interaction between regularly arranged Heisenberg or Ising spins. Generally the exchange coupling J_{ij}, which is a random variable, is assumed to be distributed according to a Gaussian curve with mean zero. Edwards & Anderson (1975) solved such a model in a generalised mean field approximation and obtained a sharp cusp in susceptibility as well as specific heat at the same temperature. However, it is well known that mean field results are not very reliable and they tend to give sharp transitions even where transitions do not exist (e.g. one-dimensional Ising model with nearest neighbour interactions). Thus it is not known whether the failure of the Edwards-Anderson model is genuine or due to the approximations involved in the calculations.

3.3b. *Monte Carlo simulation of spin glass*

Monte Carlo simulations of spin glass have been carried out by Binder & Schroder (1976a, b), Binder & Stauffer (1976) and Binder (1977) to ascertain whether the Edwards-Anderson model is suitable for describing spin glasses or whether the approximation involved in solving the model gives spurious results. Apart from the fact that Monte Carlo simulation gives better results than the mean field approximation, it also permits a study of non-equilibrium relaxation phenomenon which is of importance in spin glass systems.

Binder & Schroder considered an Ising square lattice with nearest neighbour interactions in zero and non-zero fields. The nearest neighbour interaction was chosen at random from a Gaussian distribution of width $\triangle J$ and mean zero. The quantities computed included internal energy, direct and staggered magnetisations, the spin glass order parameter $q(t)$ given by

$$q(t) = \frac{1}{N}\sum_{j=1}^{N} \left(\frac{\int_{t_i}^{t} S_j^z(t')\, dt'}{t - t_i} \right)^2, \tag{40}$$

and the autocorrelation function $\langle S_i^z(0)\, S_i^z(t) \rangle$. From these results specific heats, direct and staggered susceptibilities were computed. The internal energy is found to reach the same asymptotic value independent of the initial state while magnetisation showed remanence for a ferromagnetic initial state below T_f. The remanence showed a slow decay with time. Both the results are consistent with experimental observations. The conjecture that the autocorrelation function decays to the order parameter value as $t \to \infty$ could not be verified since the decay of the autocorrelation function is very slow. However, the order parameter q relaxed to a zero value for $k_B T > \triangle J$ but assumed a non-zero value at lower temperatures. The specific heat and susceptibility variations of a spin glass with temperature are

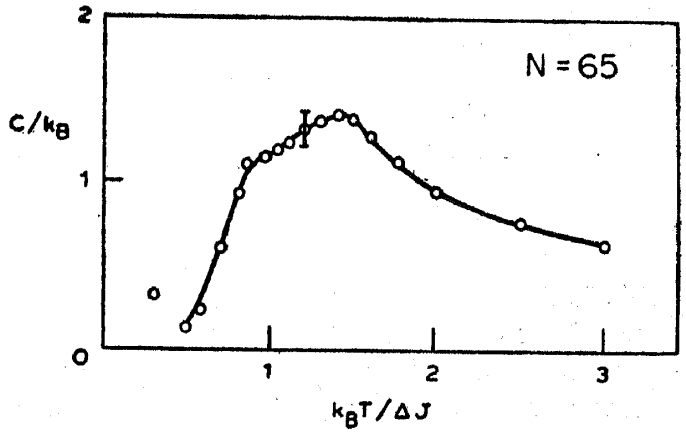

Figure 6. Specific heat vs temperature of a two-dimensional Ising spin glass. After Binder & Schroder (1976).

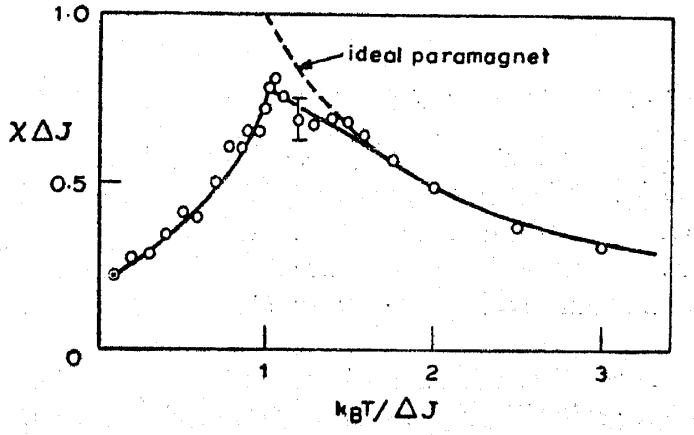

Figure 7. Susceptibility vs temperature of a two-dimensional Ising spin glass. ΔJ is the width of the Gaussian. After Binder & Schroder (1976).

shown in figures 6 and 7 respectively. We notice that the susceptibility curve shows a cusp while the specific heat curve shows a broad maxima. The temperature of the maxima is ~25% higher than the cusp temperature. The field required to smoothen the cusp in the susceptibility curve is of the same order as that predicted by the Edwards-Anderson model and is an order of magnitude higher than the required experimental fields. In the three-dimensional Ising case, the temperatures T_f and T_m come closer together. This is not surprising since for disordered systems the mean field results are known to be exact in six-dimensions.

Binder (1977) has estimated a global spin glass order parameter ψ for the Edwards-Anderson model. This order parameter is given by (Luttinger 1976)

$$\psi = \frac{1}{N}\sum_i \phi_i^{(1)} S_i^z, \tag{41}$$

where $\phi_i^{(1)}$ is the phase function for the spin glass. The phase function in the spin glass state is not known and is difficult to determine. But by using a $\phi_i^{(1)}$ obtained from the ground state spin glass simulation and using the same ground state as the initial state for calculations at non-zero temperatures, ψ has been estimated at various temperatures. The advantages of using the global order parameter ψ instead of the local order parameter q ((40)) is that ψ has a much weaker dependence on t (Monte Carlo steps/spin) than q and hence converges faster. Besides the order parameter shows critical fluctuations while q does not. The susceptibility corresponding to fluctuations in ψ diverges in the vicinity of T_f.

Thus, we see from the Monte Carlo simulation studies that the Edwards-Anderson model is a viable spin glass model and the spurious results are largely due to the generalised mean field approximations.

There has been some recent interest in the computer simulation of a real spin glass. Walker & Walstedt (1976) studied a spin glass of classical spins randomly embedded in a face-centred cubic lattice and interacting *via* RKKY interactions. However, this simulation is not a Monte Carlo simulation and it is aimed at obtaining the spin glass elementary excitation spectrum from the ground state configuration to explain the approximate linearity and concentration independence of the specific heat variation at low temperatures. De Rozario *et al* (1977) studied the ground state internal field distribution of classical spins randomly distributed on a simple cubic lattice and obtained the low temperature specific heats. This again is not a Monte Carlo simulation.

3.4. *Renormalisation group critical exponents via Monte Carlo method*

The renormalisation group method involves a study of the transformation of interaction parameters of a model under a change of length scale. This transformation gives the critical exponents of the model and this method has been very widely applied in recent times. In this subsection we shall briefly outline some exploratory attempts at obtaining this transformation by the Monte Carlo method (Ma 1976; Friedman & Felsteiner 1977).

Ma considered a two-dimensional single spin-flip kinetic Ising model. In this model, the transition probability for a spin to flip in a time interval dt is given by

$$W_i(S_i^z) = \Gamma \exp(-S_i^z B_i), \tag{42}$$

where B_i is the magnetic field seen by the spin at site i. The method adopted by Ma to obtain the transformation of interaction parameters with change of length scale is the following. Given an initial configuration S at time t, the spin-flip probabilities are computed for all the spins using (42). The probability that no spin shall flip during a period t' is given by $\exp(-\Omega t')$ where,

$$\Omega = \sum_i W_i(S_i^z). \tag{43}$$

And the probability that during a subsequent period dt', one of the spins will flip is $\Omega\, dt'$. Thus, the net probability for the two events to occur in succession is $\exp(-\Omega t')\,\Omega\, dt'$. The computational method involves (i) choosing the time t' during which none of the spins flips and (ii) choosing the site i for flipping the spin. These are chosen with the help of two random numbers x and y with $0 < x, y < 1$. The time t' is given by

$$t' = -\ln x/\Omega. \tag{44}$$

To choose i for each configuration, the interval 0 to 1 is subdivided into N sub-intervals with the length of each sub-interval proportional to W_i. The site i is now the ith sub-interval to which the random number y belongs. The spin at site i is flipped and the process of choosing t' and i are repeated for the new configuration. The quantities of interest are averaged over a large number of such cycles.

The quantities computed in this simulation are the life-times of the individual spins and block spins in different environments. Block spins are defined as spins representing the state of a block of 2×2 single spins. The block spin assumes two states, just as the single spin, depending upon the direction of magnetisation of the block with one of the four spins neglected randomly to give a net magnetisation in all situations. From the life-times of the block spins in different environments, we can calculate the interaction parameters for the block spins. The life-times of single spins serve in checking the accuracy of the calculations. The interaction parameters of the block-spins and the single spins give the elements of the matrices $\partial J'_i/\partial J_i$ and $\partial h'_i/\partial h_i$ (J'_i and h'_i are interaction parameters and fields corresponding to the interaction parameters of block spins. Similarly J_i and h_i are defined for single spins), whose eigen values are related to the critical indices. The dynamic critical exponent is related to the transformation of Γ (equation (42)). The dynamic and static critical exponents obtained from this method compare well with those obtained from other methods.

Friedman & Felsteiner (1977) have also applied the Monte Carlo technique to calculate renormalisation group critical exponents. However, they have adopted the Monte Carlo sampling technique only to estimate the partition functions of the original and the renormalisation group transformed Hamiltonians. Thus their method is not a fundamental application of the Monte Carlo method to renormalisation group transformation; they have employed the Monte Carlo method only as a numerical tool.

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