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# Microcanonical Monte Carlo study of a two-dimensional Blume–Capel model

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**Abstract.** A microcanonical Monte Carlo algorithm has been developed to calculate the density of states of a two-dimensional Blume–Capel model in zero field. The full density of states is calculated for a 16 x 16 lattice as a function of the two spin summations which appear in the Hamiltonian. This permits the partition function and related thermodynamic functions to be evaluated for any temperature and any single site anisotropy from a single data set. Results are presented for the pseudo-critical transition temperature and the maximum in the specific heat as a function of the single site anisotropy parameter. The technique will allow the region near the tricritical point to be explored in detail and will permit the future determination of the zeros of the partition function. It should be noted that the microcanonical sampling method of Lee was found to be unusably slow for the $S = 1$ problem in regions where the density of states had a significant slope and the microcanonical sampling described in this work is a significant improvement on his sampling method.

## 1. Introduction

The motivation behind the work presented in this paper is to obtain an estimate of the tricritical point in a two-dimensional ferromagnetic Blume–Capel model [1,2] by computer simulation. The problem of identifying the tricritical point, at which a phase transition moves from first order to a continuous transition, is particularly difficult in numerical simulations. A number of methods have been suggested for determining the nature of a phase transition using hysteresis [3], histogram techniques [4] and finite-size scaling [5,6]. In this work a novel microcanonical algorithm is described which allows the determination of a density of states which depends upon two terms in the Hamiltonian. This allows the partition function and thermodynamic functions to be evaluated for any temperature and any single site anisotropy. The method provides an improved technique for studying the first-order region of the phase diagram since the two parts of phase space competing in the first-order transition can be explored independently and fully. The microcanonical methods are simple to implement on a parallel array of processors since each data point in the density of states can be determined independently. The results presented here have been obtained using a 31 transputer array running as a simple processor farm.

The determination of the complete density of states for finite lattice models is also of interest in order to study the behaviour of the zeros of the partition function. The zeros in the complex plane and their finite-size scaling yield information about

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the critical properties of the system [7–14]. Thus Bhanot *et al* [7] are able to obtain an accurate value for $\nu$ in a $Z(2)$ gauge theory with a lattice of only $5^4$. The form of the finite-size scaling of the amplitude of the zero nearest to the positive real axis in the complex temperature plane yields information about the nature of the phase transition [10, 13, 15].

The work presented in this paper establishes the validity of the method for the Blume–Capel model on a $16\times16$ lattice. Future work will undertake the determination of the partition function zeros and the finite-size scaling analysis to determine the tricritical point.

The history of microcanonical methods is described in section 2, the new algorithm is described in section 3, the simulation details are given in section 4, the error analysis is given in section 5 and the results are given in section 6.

## 2. Microcanonical methods

There have been a number of studies of microcanonical Monte Carlo methods (see, for example, [7, 16–20]). The methods allow the determination of continuous thermodynamic functions from a single data set including the partition function, entropy and free energy. Lee [20] reports that in a simulation of a two-dimensional Ising model he obtained the thermodynamic functions at all temperatures for the same computational effort required to obtain a single data point in conventional Monte Carlo. However, some authors report the methods as being inefficient for more complex problems. Thus Karliner *et al* [21] suggest improvements to the method of Bhanot *et al* [7] which reintroduces Metropolis sampling over restricted energy ranges.

Other developments in conventional Metropolis Monte Carlo techniques include that of Ferrenberg and Swendsen [22, 23] who developed a histogram technique and Rickman and Phillpot [24] who developed a cumulant method. Alves *et al* have determined the density of states for an Ising model [13] and a Potts model [14] using a multiple histogram method. All these techniques enable more efficient use of the data collected by conventional Metropolis Monte Carlo methods. It should be noted that these methods have a long history as detailed in [13] and one of the earliest suggestions of a microcanonical method is that of McDonald and Singer [16].

In this work, we combine the approaches of Lee [20] and Ferrenberg [22] and develop a method which uses microcanonical sampling to determine a two-dimensional density of states. Unlike conventional Monte Carlo [25], the Hamiltonian coefficients and temperature are treated as continuous variables which are chosen after the simulation. Thus a single data set is generated which may be used to calculate continuous thermodynamic functions for a class of Hamiltonians. This makes efficient use of the simulation data.

In the following we wish to determine the density of states for a two-dimensional Blume–Capel model on a simple cubic lattice with $N$ sites and in zero external field. The standard ferromagnetic Hamiltonian is scaled by the exchange interaction, $J$, and written in the dimensionless form

$$H(S, D, \alpha) = -S + \alpha q D \tag{1}$$

where $S = \sum_{\langle i,j\rangle} \sigma_i\sigma_j$ with $\langle i, j\rangle$ = all nearest-neighbour bonds; $D = \sum_{\langle i\rangle} \sigma_i^2$ with $\langle i\rangle$ = all $N$ sites; $\sigma_i = \pm1, 0$; $q$ is the coordination number of the lattice; and $\alpha$ is a

**Table 1.** Exact values of $\rho(D, S)$ used in calculations.

| $S$ | $N$ | $N-1$ | $N-2$ | $N-3$ |
|---|---|---|---|---|
| $S_m$ | 2 | | | |
| $S_m-4$ | | $2N$ | | |
| $S_m-7$ | | | $Nq$ | |
| $S_m-8$ | $2N$ | | $N(N-q-1)$ | |
| $S_m-10$ | | $2Nq$ | | $Nq(q-1)$ |
| $S_m-11$ | | | | $Nq(N-2q)$ |

dimensionless parameter which determines the strength of the single site anisotropy. The results presented here are for a $16 \times 16$ lattice with periodic boundary conditions.

The heart of the method described here is the determination of the density of states, $\rho(S, D)$, the total number of states of the $16 \times 16$ lattice with given values of the sums $S$ and $D$. All the thermodynamic functions may then be determined from $\rho(S, D)$. Thus the canonical expectation value of any observable $\hat{O}(S, D)$ is given by

$$\langle \hat{O} \rangle = \sum_{S=-S_m}^{S_m} \sum_{D=0}^{N} \hat{O}(S, D)\rho(S, D)\exp(-\beta H(S, D, \alpha))/Z(\alpha, \beta) \tag{2}$$

where $Z(\alpha, \beta)$ is the partition function

$$Z(\alpha, \beta) = \sum_{S=-S_m}^{S_m} \sum_{D=0}^{N} \rho(S, D)\exp(-\beta H(S, D, \alpha)) \tag{3}$$

$S_m = Nq/2$ and $\beta$ is $J/k_B T$, a dimensionless inverse temperature. The parameters $\alpha$ and $\beta$ are continuous variables which are introduced during the post-processing of the simulation data.

It should be noted that $\rho(S, D)$ has the symmetry property

$$\rho(S, D) = \rho(-S, D) \tag{4}$$

and the normalization

$$\sum_{S=-S_m}^{S_m} \rho(S, D) = 2^D \, {}_N C_D \tag{5}$$

where

$${}_N C_D = \frac{N!}{D!(N-D)!} \tag{6}$$

and also that

$$\sum_{S=-S_m}^{S_m} \sum_{D=0}^{N} \rho(S, D) = 3^N \tag{7}$$

as would be expected for an $S = 1$ system.

The value of $\rho(S, D)$ may be calculated exactly for some values of $S$ and $D$. In the following we assume simply that $\rho(S, D)$ is known exactly for $|S| \geqslant S_t$. The exact values used in the results presented below are given in table 1 and it can be seen that in this work $S_t = (S_m - 11)$.

## 3. Algorithm

We define the ratio $R(S, D)$ by

$$R(S, D) = \frac{\rho(S, D)}{\rho(S+1, D)}. \tag{8}$$

In order to determine $R(S_0, D_0)$ we adopt the following algorithm:

(a) A state is generated with $D = D_0$ and with $S \in I$ where

$$I = \{S : S_L \leqslant S \leqslant S_U\}. \tag{9}$$

(b) The state is modified using an algorithm which randomly changes $S$ but not $D$. This is achieved in this work by randomly choosing a spin, $\sigma_i$. If $\sigma_i = \pm 1$, the spin value is changed in sign. If $\sigma_i = 0$, it is exchanged with a non-zero spin, $\sigma_j$, which is also chosen at random.

(c) If the new state has $S \in I$, the new state is accepted, otherwise the old state is retained.

A record is kept of the number of times, $N(S_0, D_0)$, a state with $S = S_0$ and $D = D_0$ is observed. The quantity $N(S_0 + 1, D_0)$ is also recorded. It is essential that rejected moves are included in this counting process.

The algorithm generates a Markov chain with a symmetric stochastic transition matrix and such a matrix has a left eigenvector $(1, 1 \ldots 1)$ with eigenvalue unity. Provided the matrix is irreducible this will be the limiting distribution of the Markov chain [26] and consequently

$$R(S_0, D_0) = E[N(S_0, D_0)/N(S_0 + 1, D_0)] \tag{10}$$

where $E[f]$ is the expected value of the random variable $f$.

It should be noted that it is possible to devise a very limited number of states that lie within the interval $I$ but are inacessible from the majority of the states in $I$ using the algorithm described above. This has the consequence that the matrix is reducible but the error in equation (10) is normally extremely small provided the initial state of the Markov chain is chosen to be accessible from within the interval $I$ and that $I$ is not made too narrow.

It follows from the conditions (4), (5) and (8) that for $|S| < S_t$

$$\ln[\rho(S, D)] = \ln[\rho(0, D)] - \sum_{i=0}^{S-1} \ln[R(i, D)] \tag{11}$$

where

$$\ln[\rho(0, D)] = \ln\left[2^D \, {}_N C_D - 2 \sum_{S=S_t}^{S_m} \rho(S, D)\right] - \ln\left[1 + 2 \sum_{S=1}^{S_t-1} \left\{ \prod_{i=0}^{S-1} (R(i, D))^{-1} \right\}\right]. \tag{12}$$

The choice of $I$ is central to the success of the method. This may be illustrated if we assume for simplicity that $R(S, D)$ is sensibly constant for $S \in I$ and has value $R$.

The expected number of attempted moves to obtain one state with $S = S_0 + 1$ may then be written as $N_E$ where

$$N_E = E\left[\sum_{k=-a}^{b+1} (\rho(S+k, D)/\rho(S+1, D))\right]$$
$$= \frac{1}{R^b}[(R^{a+b+2} - 1)/(R - 1)] \tag{13}$$

where

$a$ = number of allowed states with $S \in \{S : S_L \leqslant S < S_0\}$

$b$ = number of allowed states with $S \in \{S : S_0 + 1 < S \leqslant S_U\}$.

In the spin-$\frac{1}{2}$ model considered by Lee [20], a choice of $a = b = 2$ ensures that all attempted moves starting in the algorithm from states with either $S = S_0$ or $S = S_0 + 1$ are successful. Lee argues that this maximizes the statistical efficiency of method. Unfortunately in the spin-1 model, the states are more densely packed in S and it is necessary to choose $a = b = 8$ in order that all moves from either $S = S_0$ or $S = S_0 + 1$ are successful. In this case, $N_E$ becomes $O(R^9)$ rather than $O(R^3)$ for Lee's model.

## 4. Simulation details

In the results presented below, we choose $a = 0$ and $b = 8$. This has the consequence that many of the attempted moves from $S = S_0$ or $S = S_0 + 1$ are rejected but $N_E$ becomes $O(R)$. Clearly, when $R$ is large, the majority of trial states will have the lower values of $S$ and the method will not generate new states very efficiently. However, the method generates new states much more rapidly than $O(R^9)$ and consequently the method is a considerable improvement over that of Lee's.

The $N(S_0, D_0)$ follow a binomial distribution and the efficiency with which the system generates independent configurations can be estimated within the simulation by calculating a statistical inefficiency (e.g. [27]). The inefficiency, $\tau$, is defined to be the ratio of the observed variance in $N(S_0, D_0)$ to the variance expected on the assumption of uncorrelated binomial statistics. It can be shown that this is given by

$$\tau = \frac{p}{1-p} N_{tot} f^2 \tag{14}$$

where $p$ is the probability of the system being in state $N(S_0, D_0)$, $N_{tot}$ is the total number of attempted spin flips for the determination of $R(S_0, D_0)$ and $f$ is the fractional error in $N(S_0, D_0)$. The quantity $p$ was estimated by $N(S_0, D_0)/N_{tot}$ and $f$ was estimated by dividing the data into ten sub-blocks. For each calculation of $R(S_0, D_0)$ the simulation was run for an 'equilibration period' during which time a preliminary value for $\tau$ was calculated. This was then used to estimate the number of flips needed to achieve the target fractional error and an appropriate data collection run was then implemented. The fractional error during the data collection run was measured to verify the choice of number of spin flips. The validity of the statistical

assumptions used in the derivation of equation (14) was verified by the success of this method in predicting correctly the number of flips needed to achieve a required fractional error over a wide range of values of $R(S_0, D_0)$.

The variation of the inefficiency $\tau$ with $S$ value are presented in figure 1 for the cases $D = 256$ in the $16 \times 16$ lattice and $D = 484$ in the $22 \times 22$ lattices. In each figure the results are collected from ten independent runs each with a target fractional error of $f = 0.01$. These two cases correspond to $S = \frac{1}{2}$ Ising models. It can be seen that the inefficiency rises to a broad maximum around the critical region of this spin-$\frac{1}{2}$ system. However, the number of spin flips per site to achieve an independent state is approximately 3.1 for the $16 \times 16$ lattice and 1.7 for the $22 \times 22$ for the broad set of states near the critical point. This is similar to the efficiency achieved with cluster flip algorithms [29] and on the basis of this limited data it appears that $\tau$ scales with the lattice size $L$ as $L^z$ with $z < 1$. This result is consistent with that reported by Bhanot *et al* [7] who suggest that the microcanonical method does not suffer from conventional critical slowing down.

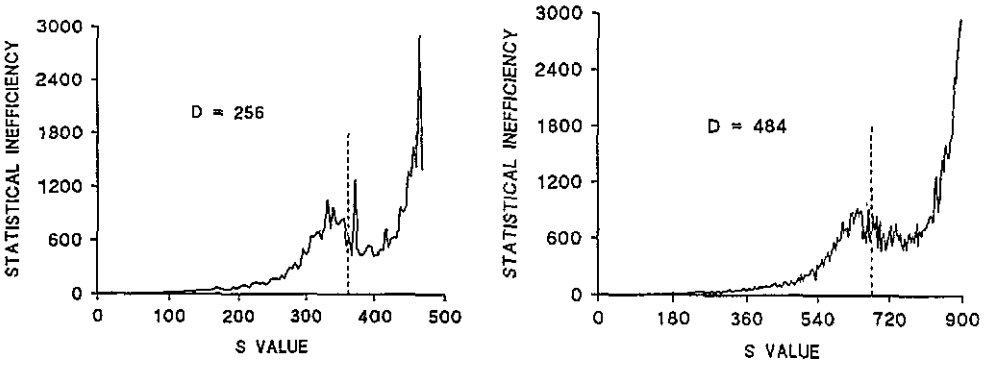


**Figure 1.** Statistical inefficiency,$\tau$, as a function of $S$ value for $D = 256$ and $D = 484$. In each diagram the value of $S$ at the centre of the critical region is marked with the dotted vertical line.

A possible reason for the difference from conventional critical dynamic behaviour is that the dynamics of the method is determined by a correlation function of the form $\langle R(0)R(t)\rangle$, where $R$ is the ratio defined in equation (10), rather than an order parameter correlation function. Further, the microcanonical method works on an energy 'window' which does not change with lattice size although the fluctuations $(\delta E)^2$ increases with box size. Thus the method only samples a limited number of the critical states in each microcanonical run. Since a critical system does not exhibit a *critical energy* it is possible that a microcanonical simulation will not exhibit conventional critical slowing down as seen in standard Monte Carlo simulations near to second-order phase transitions. However, it should be noted that the value of $\tau$ does become very large for the regions of $\rho(S, D)$ with values of $R \simeq 10^2$.

The technique has been further proved by successfully calculating $R(S, D)$ for values of $S \geqslant S_t$ where $R(S, D)$ is known exactly and has values of a few hundred. The success of the method in these regions is a very significant improvement over the method of Lee which became unusably slow in this problem even for values of $R(S, D)$ close to 2. The choice of $b = 8$ ensures that any spin flip which increases

$S$ from $S_0 + 1$ will always be accepted. If $b$ is chosen to be too small, there will be a problem with ergodicity as explained above. The success of the method for values of $S \geqslant S_t$ suggests that the current method is ergodic.

The technique described above has been implemented on a transputer array of 31 transputers. The code was written in parallel C and the algorithm for calculating $R(S, D)$ described in the algorithm (a) to (c) was implemented as a worker process within a flood fill configurer. The method, therefore, gives a parallel Monte Carlo program with a speed of computation which scales linearly with the number of processors.

The average time taken for one attempted spin flip was 43 $\mu$s and hence with 31 processors the effective time for a spin flip was 1.4 $\mu$s. The data presented below were collected over a period of 12 days and represent approximately $10^{12}$ attempted spin flips in total. This represents approximately $4 \times 10^9$ lattice sweeps. Tucker [28] has reported requiring approximately $10^7$ lattice sweeps to obtain the tricritical point to a similar accuracy reported in this paper using conventional Monte Carlo histogram techniques [22]. However, these results only cover a limited range of $\alpha$. The code has not been optimized and further speed improvements could be achieved by writing the core of the algorithm in a low-level language. Bhanot *et al* [18] show that the simulation time to determine a one-dimensional density of states to a given maximum error in each value of the density of states, scales as $V^2$ using this type of microcanonical method, where $V = L^d$. The simulation time to determine a two-dimensional density of states to a given accuracy using the method described in this paper will scale as $V^3$. This arises because the density of states is essentially calculated along lines of constant D, the number of such lines scales as $V$ and the simulation time for each line scales as $V^2$, as in the Bhanot case. However, in determining a thermodynamic function from the density of states, the density is summed over a set of points whose number scales as $L^2$. The simulation time to determine a thermodynamic function to a given accuracy will therefore scale as $V^3/L$.

## 5. Error estimates

As explained above, the algorithm was designed to obtain each $N(S_0, D_0)$ with a fractional error $f = 1\%$ as measured from the sample variance. The error in the $R$ values is $\sqrt{2}f$ and the maximum absolute error in $\rho(S, D)$ is determined by the propagation of the errors in the individual $R$ values and is given for an $L \times L$ system by

$$f_{\max} = \sqrt{q} L f. \tag{15}$$

In our work this corresponds to a maximum fractional error in $\rho(S, D)$ of 32%. However, in the calculation of the specific heat from the density of states the number of $\rho(S, D)$ values which make a significant contribution will be of the order $kL^2$ where, by inspection of the data, $k$ is at least four. Thus the fractional error in the specific heat will be $f_C = 1\%$. As explained below, the transition temperature is determined from the maximum in the specific heat. The error in the transition temperature is therefore determined by the error in the specific heat, $C$, and also the value of $\partial C/\partial T$ at the maximum. From an inspection of the specific heat results, the maximum error in the transition temperature is 0.4% with an error of 0.15% near to the tricritical region.

These arguments were checked by considering the $D = 256$ data which correspond to a spin-$\frac{1}{2}$ model for which exact results are known for a finite lattice [30]. The data gave the normalization of equation (5) to an accuracy of 5% which is consistent with a predicted error of 16%. The specific heat was determined to 0.9% of the analytic value and the transition temperature to 0.4% of the analytic value, against predicted errors of 1% and 0.5% respectively. It should be noted that this data set took $1.5 \times 10^6$ lattice sweeps to accumulate.

It is important that the Boltzmann factor $\exp(-\beta H)$ associated with each term in the summation (2) is calculated explicitly for each value of $S$ and $D$. Thus in initial calculations of the specific heat, a histogram of the density of states in energy for given alpha was constructed and this was then used to generate an energy probability distribution at a given temperature by multiplying each term in the histogram by an appropriate Boltzmann factor. Unfortunately, the quantization in energy required to construct the histogram was reflected in small discontinuities in the graph of critical temperature against alpha. It is probable that similar 'quantization noise' will be experienced in using histogram techniques (e.g. [22,23]) with conventional Monte Carlo techniques.

In the future determination of the partition function zeros, the partition function will be written as

$$Z(x,y) = \sum_{S=-S_m}^{S_m} \sum_{D=0}^{N} \rho(S,D) x^S y^D \tag{16}$$

where $x = \exp(\beta)$ and $y = \exp(-\beta\alpha q)$. The zeros of $Z$ can be determined either in the complex $x$ or complex $y$ plane. In each case the coefficients of the associated polynomial will be determined by a summation over a set of $\rho(S,D)$ values. The principal contribution to each coefficient will come from a set of values whose number is of order $L$ and this will reduce the error for the coefficients from that given in equation (15). The error in the zero nearest the real axis is considerably less than the error in the coefficients in the polynomial [18] but it will be necessary to reduce the errors further in order to obtain adequate scaling results. This will be achieved by longer runs and by modifing the algorithm to make more effective use of the observed data. It should be noted that the calculation of the two-component density of states for this spin-1 model on a $16 \times 16$ lattice is as computationally demanding as determing the full density of states for a spin-$\frac{1}{2}$ model on a three-dimensional lattice of size $22 \times 22 \times 22$.

## 6. Results

The observed density of states is shown in figure 2 for $S \geqslant 0$ but it should be noted that the plotting algorithm is unable to show fine structure in the density of states. For example, along the line $D = 256$ the system is effectively spin-$\frac{1}{2}$ and the density of states is only non-zero when $S$ is divisible by four. However these 'fjords' in the density of states are not resolved by the plotting algorithm.

The region of large $S$ and $D$ corresponds to the ordered ferromagnetic phase. The region of small $S$ and $D$ corresponds to the 'disordered', paramagnetic phase. A line of constant energy is also shown in figure 2. It can be seen that, when $\alpha$ is

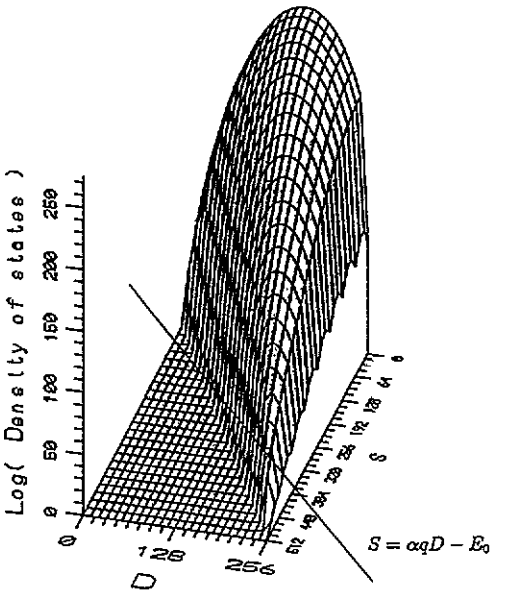


**Figure 2.** Density of states $\rho(S, D)$ in the Blume–Capel model for a 16 x 16 lattice; line of constant energy $E_0$ for $\alpha \approx 0.5$.

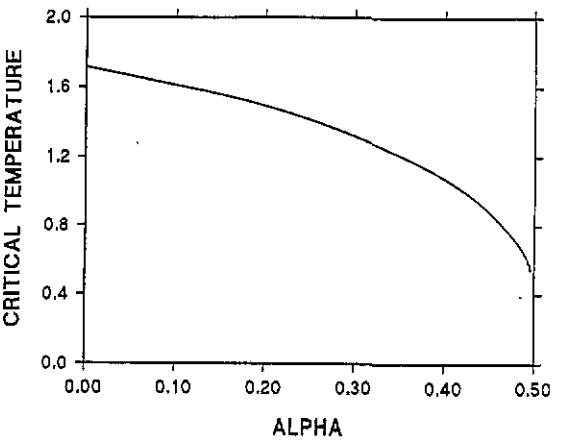


**Figure 3.** Pseudo-critical transition temperature determined from the peak in specific heat in the 16 x 16 two-dimensional Blume–Capel model. Temperature in reduced units $k_B T/J$.

approximately 0.5, the system is exploring both regions and it is these two parts of the phase space which will contribute to the first-order behaviour.

The density of states has been used to calculate the specific heat from the fluctuations in the energy and as a function of $\alpha$ and $\beta$. Figure 3 shows the pseudo-critical temperature $T_c(L)$ where $L$ is the linear dimension of the lattice. The value of $T_c$ presented in figure 3 is obtained from the maximum in the specific

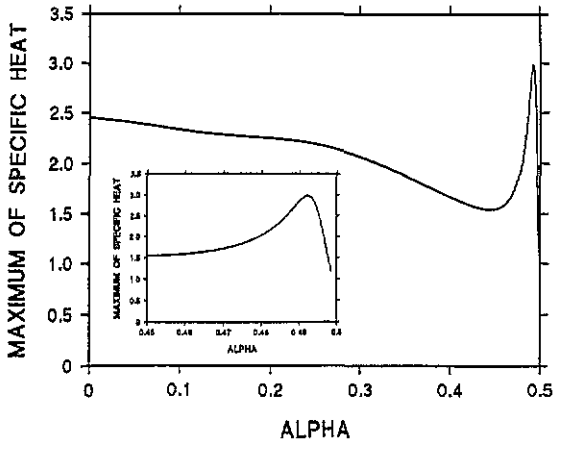


**Figure 4.** Maximum value of specific heat as a function of the single site anisotropy parameter, $\alpha$, in the two-dimensional Blume–Capel model on a 16 x 16 lattice. Specific heat equivalent to heat capacity per spin in reduced units of $C/k_B$

heat for $L = 16$. Figure 4 shows the maximum value in the specific heat calculated from density of states for a range of values of $\alpha$. The specific heat maximum has a maximum as a function of $\alpha$ for a value $\alpha = 0.4924 \pm 0.0025$ and temperature $T = 0.5969 \pm 0.0008$. It is assumed that this peak is related to the onset of first-order behaviour above the tricritical temperature since it is known from the mean-field calculations [1,2] that the phase transition becomes first order for $\alpha$ just less than 0.5. The results are close to the values for the tricritical point calculated by Monte Carlo renormalization group and other methods [31–34].

The change from first-order transition to continuous transition near the tricritical point can be also studied by considering the probability of the system having a given energy. In a first-order region, this probability function exhibits the double-peak structure [4] as seen in figure 5, and this should not disappear [5] as the box size

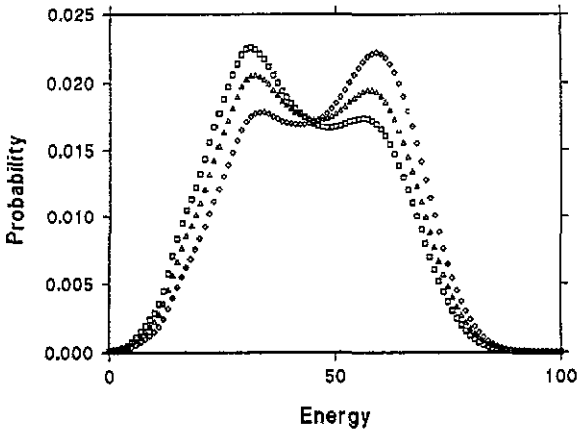


**Figure 5.** Probability of energy in Blume–Capel model with $\alpha = 0.491$ and energy in reduced units of $E/J$: ◇, $\beta^{-1} = 0.615$; △, $\beta^{-1} = 0.611$; □, $\beta^{-1} = 0.608$

$L \to \infty$. The two-peak probability distribution and the tricritical behaviour are related to the geometrical structure of the density of states for large $L$ and the way in which the two wings of the surface are explored for given $\alpha$ by $\exp(-\beta(-S + \alpha q D))$. The relative weight of the two peaks changes as the temperature of the system is increased and the two peaks merge as the value of alpha is reduced from 0.5.

## 7. Summary

In conclusion the microcanonical Monte Carlo method described above has the merit of being straightforward to parallelize and explores both regions of a first-order transition independently. The method does not appear to exhibit conventional critical dynamics seen in standard Monte Carlo simulations of second-order phase transitions. It was found that the microcanonical sampling method of Lee was unusably slow for the $S = 1$ problem in regions where the density of states had a significant slope and the microcanonical sampling described in this work is an improvement of his sampling method. The method will also improve on that of Bhanot *et al* [15, 18, 19] in regions where the slope of the density of states is large. The method gives results for the complete range of temperature and single site anisotropy parameter, $\alpha$, and allows calculation of the partition function zeros. However, the computational effort depends upon the box dimensions as $V^3/L$ and this is a serious limitation. The modifications suggested by Karliner *et al* [21] of introducing Metropolis Monte Carlo within bounded energy may improve the simulation time but possibly at the expense of the return of conventional critical dynamics. The method in its present form is restricted to lattice problems and its main value may be in exploring systems which exhibit first-order transitions.

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