Microcanonical ensemble Monte Carlo method for discrete systems

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In an earlier work [Phys. Rev. A **44**, 4061 (1991)] a method of carrying out Monte Carlo simulations in the microcanonical ensemble was discussed and applied to systems described by continuous potentials. This method can also be used for discrete systems, e.g., spin, lattice gas, or alloy type models where it furnishes a different way of exploring the system than the canonical ensemble. A complete statistical mechanics and related thermodynamics exists for this microcanonical ensemble. We give microcanonical ensemble fluctuation formulas for the specific heat and constant energy susceptibility and relate these to the analogous canonical ensemble expressions for the Ising model. As an example we present simulation results for a two-dimensional Ising model and compare the microcanonical and canonical ensemble calculation of various physical properties of the system. An interesting feature is the appearance of a large (16%) ensemble difference between the specific heat in canonical and microcanonical ensemble simulations for a 30×30 Ising system in the vicinity of the maximum in the specific heat.

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I. INTRODUCTION

Following the introduction of the canonical ensemble Monte Carlo method into statistical mechanics by Metropolis *et al.* [1] most Monte Carlo simulations have used the canonical ensemble. Recently [2] we discussed a microcanonical ensemble Monte Carlo procedure and applied it to systems described by a continuous potential. We have also developed other constant energy ensembles and carried out Monte Carlo simulations in these ensembles; these include the isoenthalpic-isotension ensemble [3], and other ensembles that describe open systems [4].

Since the microcanonical ensemble describes an isolated system this ensemble is at least as fundamental as the canonical ensemble but has, inappropriately, been neglected in simulation work since the canonical ensemble is more popular in analytic work where it is usually much simpler to use; in simulations there is no difference in difficulty between using the canonical or microcanonical ensembles.

Other microcanonical simulations of discrete systems employ the microcanonical simulation method of Cruetz [5], which is, however, not a Monte Carlo method but a deterministic procedure. Because Cruetz's method involves only integer variables and no random numbers one can make very efficient programs using this procedure, and this property has been exploited by various workers [6–8]. Other simulations of discrete systems have been carried out using Cruetz's method including the works of Harris [9], Gould and Tobocnik [10], and Heermann [11]. Cruetz's microcanonical simulation method applied to discrete systems makes use of a plausible algorithm to equilibrate a system under conditions of constant energy, where the energy is the sum of the systems potential energy and the energy of a demon that is introduced into the algorithm. Although the Cruetz method has certain advantages, such as efficiency, it does not appear to have a rigorous basis in statistical mechanics and apparently cannot be used to directly (i.e., using fluctuation formulas) calculate thermodynamic response function such as specific heats, susceptibilities, etc. in the microcanonical ensemble.

In this paper we discuss and illustrate the microcanonical ensemble simulation method applied to discrete systems. Since this microcanonical ensemble method is rigorously based in statistical mechanics we can calculate anything that can be calculated in the canonical or any other ensemble. We shall give the basic fluctuation formulas for the specific heat and susceptibility and relate these to the analogous relations in the canonical ensemble for the Ising model. We shall present detailed results of simulations of a 30×30 Ising spin system in zero magnetic field and give some results for a 60×60 system in both the canonical and microcanonical ensembles.

II. DIFFERENT ENSEMBLES

A. General discussion

In a Monte Carlo simulation one carries out a Markovian random walk through the space of system configurations such that the configurations that are generated have the probability distribution of the ensemble employed. In the thermodynamic limit ($N, V\rightarrow\infty, N/V\rightarrow$finite) different ensembles in general produce equivalent results. However, for finite systems, such as used in many-body simulations, there are finite size effects that can lead to differences in physical quantities in different ensembles. For example, the thermodynamic variables that are held fixed in a particular ensemble are ensemble dependent, as are the basic fluctuation formulas that can be used for calculating thermodynamic response functions. We shall show a dramatic example of ensemble dependence of the specific heat in a

two-dimensional Ising model where there is a 16% difference in the specific heats calculated in the canonical and microcanonical ensembles near the maximum value. This large ensemble difference is a precursor of the phase transformation of the system in the thermodynamic limit.

It has been conjectured that fixing the energy rather than the temperature should permit, for example, a more detailed study of the coexistence region in first order phase transformations [12], although this has been questioned by Brown and Yegulalp [13]. It is sometimes stated that the rate of approach of a system to equilibrium may be influenced by the particular ensemble employed. Below we shall summarize a few results from the canonical and microcanonical ensembles and later compare simulation results from these two ensembles for the same system, and two-dimensional Ising model in zero magnetic field.

B. Canonical ensemble

The canonical ensemble is described by a probability density in phase space $W_c(p,s)$, where p represents the momenta of the N particles and s represents the configuration variables that in this case are the spin of each particle,

$$W_c(p,s)=Ae^{-H(p,s)/(k_BT)}, \tag{1}$$

where $H=K(p)+U(s)$ is the system Hamiltonian, $K(p)$ the kinetic energy, $U(s)$ the potential energy, and A a constant. Although often we do not think of the particles in a discrete system, such as an Ising model, as having a kinetic energy, we can imagine the spin is associated with particles with momentum p which have a very large mass so that there is no spatial motion of the particles. Integrating over the momenta then leads to the configuration probability density

$$W_T(s)=A'e^{-U(s)/(k_BT)}, \tag{2}$$

where A' is another constant. The Metropolis Monte Carlo acceptance probability is $W(s\rightarrow s')=\min[1,W_T(s')/W_T(s)]$ with $W_T(s)$ given by Eq. (2). In the present applications we generate trial states s' by going through all the spins in sequence. The state s' differs from s by one spin being inverted and the acceptance or refection of this trial state is determined by the Metropolis probability given above.

The average value of any quantity $A(s)$ can be determined using the probability density $W_T(s)$ as

$$\langle A\rangle=\frac{\sum_{\{s\}}W_T(s)A(s)}{\sum_{\{s\}}W_T(s)}, \tag{3}$$

where $\sum_{\{s\}}$ represents a sum over all spin configurations. The canonical ensemble Metropolis Monte Carlo method is a procedure for evaluating (estimating) the average values in Eq. (3). The average energy of the system is

$$\langle E\rangle=\frac{dNk_BT}{2}+\langle U\rangle, \tag{4}$$

where d is the spatial dimension of the system and the temperature T is an input parameter. For simplicity in writing down the fluctuation formulas we consider a d-dimensional Ising model defined by the potential energy $U(s)$,

$$U(s)=-J\sum_{\langle ij\rangle}S_iS_j-B\sum_i S_i, \tag{5}$$

where J is the spin-spin coupling constant and B is the external magnetic field; we have chosen units such that J and B are in units of energy and the notation $\langle ij\rangle$ indicates a sum over distinct nearest neighbor interactions. The magnetization of the system is defined as the negative derivative of $U(s)$ with respect to B, $M=-[\partial U(s)/\partial B]$, with the average of M being the thermodynamic magnetization of the system. The configuration heat capacity $C=(\partial\langle U\rangle/\partial T)_B$ and the isothermal susceptibility $\chi_T=(\partial\langle M\rangle/\partial B)_T$ can be evaluated from the canonical ensemble fluctuation formulas

$$C=\frac{1}{k_BT^2}(\langle U^2\rangle-\langle U\rangle^2) \tag{6}$$

and

$$\chi_T=\frac{1}{k_BT}(\langle M^2\rangle-\langle M\rangle^2), \tag{7}$$

which may be derived by direct differentiation [10].

C. Microcanonical ensemble

The microcanonical probability density $W_m(p,s)$ has a constant value on the energy shell $H(p,s)=E$, where H is the system Hamiltonian

$$W_m(p,s)=D\delta(E-H(p,s)), \tag{8}$$

where D is a constant and δ represents the Dirac delta function. By integrating Eq. (8) over the momenta we obtain the configuration probability density for the microcanonical ensemble $W_E(s)$[2],

$$W_E(s)=D'(E-U(s))^{(dN/2)-1}\Theta(E-U(s)), \tag{9}$$

where d is the spatial dimension of the system, $\Theta(x)$ is the unit step function that is 1 for $x>0$ and zero otherwise, and D' is another constant; the Θ function arises because the kinetic energy of the system $K=E-U$ is positive. The Monte Carlo acceptance probability is $W(s\rightarrow s')=\min[1,W_E(s')/W_E(s)]$ with $W_E(s)$ given by Eq. (9). The trial states are generated by going through the spins in sequence and attempting to invert the spins one at a time. The acceptance or rejection of the trial state is determined by the Metropolis rules.

The microcanonical ensemble average value of any quantity $A(s)$ can be determined using the probability density $W_E(s)$ as

$$\langle A\rangle=\frac{\sum_{\{s\}}W_E(s)A(s)}{\sum_{\{s\}}W_E(s)}, \tag{10}$$

where $\sum_{\{s\}}$ represents a sum over all spin configurations.

The microcanonical ensemble Monte Carlo method is a procedure for evaluating (estimating) the averages in Eq. (10). The average value of $E-U(s)$ is the kinetic energy $\langle K\rangle=\langle E-U(s)\rangle=E-\langle U(s)\rangle$ and we use this to define the system temperature via

$$dNk_BT/2=\langle K\rangle\ . \tag{11}$$

For simplicity in writing down the fluctuating formulas we again consider a d-dimensional Ising model defined by the potential energy $U(s)$. Differentiating T in Eq. (11) with respect to E at constant B we obtain the fluctuation formula for the heat capacity $1/C_B=(\partial T/\partial E)_B$,

$$\frac{dNk_B}{2C_B}=\frac{dN}{2}-\left[\frac{dN}{2}-1\right]\langle K\rangle\left\langle\frac{1}{K}\right\rangle\ , \tag{12}$$

where the appearance of the average of the inverse kinetic energy ($K=E-U$) arises directly from the form of the probability distribution Eq. (9) for an energy shell ensemble. Note that the heat capacity C_B contains the ideal gas contribution, $C_B=dNk_B+C$, where C is the configuration heat capacity. Equation (12) should be compared with Eq. (6) in the canonical ensemble. Note that in the canonical ensemble C is directly related to the fluctuations in the potential energy but in the microcanonical ensemble this is no longer the case; one cannot reduce Eq. (12) to contain only U and not E or K.

The microcanonical ensemble fluctuation formula for the constant energy susceptibility $\chi_E=(\partial\langle M\rangle/\partial B)_E$ is given by

$$\chi_E=\left[\frac{dN}{2}-1\right]\left[\left\langle\frac{M^2}{K}\right\rangle-\langle M\rangle\left\langle\frac{M}{K}\right\rangle\right]\ , \tag{13}$$

which we derive by differentiating $\langle M\rangle$ with respect to B at constant E. Equation (13) should be compared to Eq. (7); note, however, that these two susceptibilities are not the same quantity since they are defined by holding different quantities constant; T for the canonical ensemble and E for the microcanonical ensemble. By using thermodynamic relations we can establish the following connection between the constant energy and isothermal susceptibilities:

$$\chi_T=\chi_E+\left[\frac{dN}{2}-1\right]\left[\left\langle\frac{M}{K}\right\rangle-\langle M\rangle\left\langle\frac{1}{K}\right\rangle\right]\left[\frac{2C_B}{dNk_B}\right]$$
$$\times\left\{\left[\frac{dN}{2}-1\right]\langle K\rangle\left\langle\frac{M}{K}\right\rangle-\frac{dN}{2}\langle M\rangle\right\}\ , \tag{14}$$

where all quantities on the right-hand side are evaluated in the microcanonical ensemble. Equation (14) allows us to calculate the isothermal susceptibility in a microcanonical ensemble simulation from the constant energy susceptibility. Of course, it is also possible to calculate the constant energy susceptibility from the isothermal susceptibility in the canonical ensemble; for completeness we give the formula

$$\chi_E=\chi_T-\frac{1}{C_Bk_BT^2}(\langle MU\rangle-\langle M\rangle\langle U\rangle)$$
$$\times\left[\frac{1}{k_BT}(\langle MU\rangle-\langle M\rangle\langle U\rangle)-\langle M\rangle\right]\ , \tag{15}$$

where all quantities on the right-hand side of Eq. (15) are evaluated in the canonical ensemble.

III. SIMULATION RESULTS

We constructed programs to study the two-dimensional Ising model using either the canonical or microcanonical ensemble. Periodic boundary conditions were used in all simulations. We shall present detailed data for a 30×30 spin system in zero magnetic field. Each spin can either be up $(+1)$ or down (-1) and the system is described by the potential energy of Eq. (5) with $B=0$. We shall measure the energy in units of J and the temperature in units of k_BT/J so that all quantities we quote will be dimensionless. The pseudorandom number generator RANMAR developed by Marsaglia, Zaman, and Tsang [14] and discussed by James [15] was employed; a few calculations were carried out for checks using other random number generators. For the canonical ensemble we selected nine temperatures from 1.5 to 3.0. The results we found for quantities in the canonical ensemble are consistent with published results for this system. The phase transformation in the thermodynamic limit (Onsager's solution) occurs at a temperature of approximately 2.269. We equilibrated the system at each of the nine temperatures for at least 5×10^6 Monte Carlo moves, where a Monte Carlo move consists of separate attempts to invert each of the 900 spins in the lattice in sequence. Thus, each move consists of 900 Metropolis

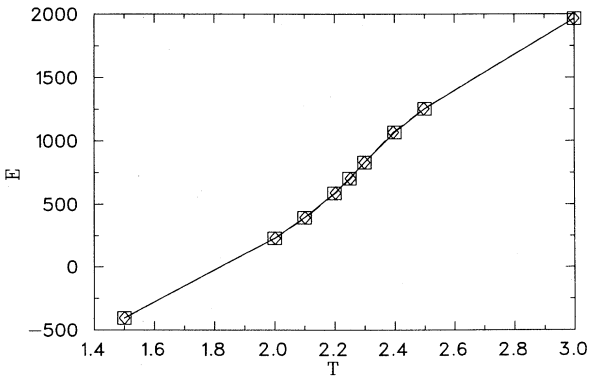

FIG. 1. Energy vs temperature for the nine simulations. The solid line and the squares are the canonical ensemble values and the diamonds and dashed line are the microcanonical ensemble values. The lines are just to guide the eye. Note the dashed line is not apparent in this figure due to the close agreement between the values in the two ensembles. The values used to make these graphs are shown in Tables I and II.

TABLE I. Canonical ensemble Monte Carlo temperature, average total energy, average absolute value of the magnetization divided by the maximum absolute value of the magnetization (i.e., 900 for the 30×30 lattice), average potential energy divided by the minimum possible value of the potential energy (-1800), and the specific heat for the 30×30 Ising model. All the quantities are dimensionless. The average values were determined by carrying out five simulations of 1×10^6 moves and averaging the five numbers obtained. Using the values from these five simulations the standard deviation was determined as an uncertainty or error estimate. These error estimates are given below each value. The temperature is an input value and has no uncertainty.

T	$\langle E\rangle$	$\langle\lvert M\rvert\rangle/\lvert M_0\rvert$	$\langle U\rangle/U_0$	c
1.500	−406.02	0.98 650	0.97 557	0.19 723
	(1.3×10^{-2})	(4.5×10^{-6})	(8.9×10^{-6})	(2.2×10^{-4})
2.000	229.00	0.91 132	0.87 278	0.72 530
	(1.1×10^{-1})	(9.1×10^{-5})	(6.3×10^{-5})	(2.0×10^{-3})
2.100	394.09	0.86 876	0.83 106	0.96 278
	(1.3×10^{-1})	(2.2×10^{-4})	(7.4×10^{-5})	(1.8×10^{-3})
2.200	587.74	0.78 587	0.77 348	1.3950
	(3.8×10^{-1})	(7.3×10^{-4})	(2.1×10^{-4})	(7.6×10^{-3})
2.250	703.09	0.70 263	0.73 439	1.72 195
	(6.1×10^{-1})	(1.6×10^{-3})	(3.4×10^{-4})	(8.4×10^{-3})
2.300	829.94	0.57 900	0.68 892	1.8712
	(6.3×10^{-1})	(2.1×10^{-3})	(3.5×10^{-4})	(4.4×10^{-3})
2.400	1066.83	0.33 282	0.60 732	1.3026
	(1.6×10^{-1})	(7.9×10^{-4})	(8.9×10^{-5})	(3.9×10^{-3})
2.500	1253.00	0.21 454	0.55 389	0.89 491
	(8.4×10^{-2})	(3.0×10^{-4})	(4.7×10^{-5})	(1.2×10^{-3})
3.000	1964.52	0.09 080	0.40 860	0.40 124
	(8.6×10^{-2})	(1.6×10^{-4})	(4.8×10^{-5})	(8.3×10^{-4})

Monte Carlo decisions on trial single spin inversions. After the equilibration period we carried out five 1×10^6 move canonical ensemble Monte Carlo simulations to collect various averages at each temperature; the five values are used to estimate an uncertainty or error estimate in each average value by calculating the standard deviation.

From the average potential energy $\langle U\rangle$ in the canonical ensemble simulations we use Eq. (4) to calculate the energy E to be used in the microcanonical ensemble simulations. From the nine canonical ensemble simulations at different temperatures we determine nine ener-

TABLE II. Microcanonical ensemble Monte Carlo average temperature, total energy, average absolute value of the magnetization divided by the maximum absolute value of the magnetization, average potential energy divided by the minimum possible value of the potential energy, and the specific heat. All the quantities are dimensionless. The average values were determined by carrying out five simulations of 1×10^6 moves and averaging the five numbers obtained. Using the values from these five simulations the standard deviation was determined as an uncertainty or error estimate. The energy is an input value and has no uncertainty. These error estimates are given below each value.

$\langle E-U\rangle/N=T$	E	$\langle\lvert M\rvert\rangle/\lvert M_0\rvert$	$\langle U\rangle/U_0$	c
1.5005	−406.00	0.98 667	0.97 581	0.19 576
(1.7×10^{-5})		(5.6×10^{-6})	(8.4×10^{-6})	(2.6×10^{-4})
2.0014	229.00	0.91 267	0.87 348	0.71 799
(3.0×10^{-5})		(1.6×10^{-5})	(1.5×10^{-5})	(2.1×10^{-3})
2.1086	394.08	0.86 805	0.82 872	0.97 132
(9.6×10^{-5})		(1.2×10^{-4})	(4.8×10^{-5})	(2.9×10^{-3})
2.2031	588.20	0.79 586	0.77 477	1.3632
(1.5×10^{-4})		(3.3×10^{-4})	(7.4×10^{-5})	(6.9×10^{-3})
2.2531	703.09	0.72 056	0.73 594	1.7727
(1.6×10^{-4})		(8.7×10^{-4})	(8.0×10^{-5})	(1.5×10^{-2})
2.2997	829.94	0.58 828	0.68 879	2.1707
(2.3×10^{-4})		(1.1×10^{-3})	(1.2×10^{-4})	(3.1×10^{-2})
2.3957	1066.00	0.31 710	0.60 562	1.2687
(7.7×10^{-5})		(1.4×10^{-3})	(7.7×10^{-5})	(3.6×10^{-3})
2.4977	1253.00	0.20 657	0.55 273	0.87 424
(5.7×10^{-5})		(6.4×10^{-4})	(2.8×10^{-5})	(2.7×10^{-3})
2.9984	1964.00	0.09 194	0.40 814	0.40 004
(7.1×10^{-5})		(8.7×10^{-5})	(3.5×10^{-5})	(1.3×10^{-3})

gies, which were then input into the probability density for the microcanonical ensemble, Eq. (9). We then equilibrated the system at the nine different energies for at least 5×10^6 moves using the microcanonical ensemble Monte Carlo method. After this equilibration period we carried out five 1×10^6 move microcanonical ensemble simulations, to collect various averages at each energy and to obtain an estimate of the uncertainty in the values.

In Fig. 1 we show the total energy E versus temperature values T for the two different ensembles for the nine different energies/temperatures. The squares are the canonical ensemble values while the diamonds are the microcanonical ensemble values. In the canonical ensemble the energy is the calculated value, whereas in the microcanonical ensemble it is the temperature that is the calculated value. As is clear in Fig. 1 there is very close agreement between the values of E,T between the two ensembles. This further supports our suggestion that either of the two ensembles can be used to study the system. There are ensemble differences in the average values of quantities for finite systems [16]. For the energy we may use Eq. (2.10) of Ref. [16] to find the relation $E_m=E_c$, where E_m is the energy in the microcanonical ensemble, E_c is the average energy in the canonical ensemble. The energies are shown in Tables I and II.

In Fig. 2 we show the dimensionless configuration specific heat, $c=C/Nk_B$, calculated in the two ensembles. The two specific heats show close agreement except near the maximum, $T\approx2.30$ where c(microcanonical $=2.1707\pm0.03$, while c(canonical) $=1.8712\pm0.004$. This large ensemble difference in specific heats is due to incipient phase transformation in the model. Note that in the thermodynamic limit (Onsager's solution) the specific heat is divergent at the transition temperature. In Fig. 3 we show a more detailed view of the region near the maximum in Fig. 2. Note that the specific heats arise from the first derivative of the energy verses temperature curves shown in Fig. 1. We use the fluctuation formulas to determine the first derivative of these curves directly, but it would be very difficult to accurately determine the specific heats in the vicinity of the maximum by numerical differentiation of the energies in Fig. 1. This shows the power of using fluctuation formulas in this region. It is possible that this large difference between quantities calculated in different ensembles could be useful in searching for or characterizing the nature of phase transformations in other systems. A (higher order) phase transformation would be characterized by when the ensemble difference between (intensive) physical quantities is much greater than $O(1/N)$; in our case this is 16% compared to around 0.1%. Much more work would have to be done to see if this is a useful procedure.

We also carried out some calculations on a 60×60 lattice near the maximum in the specific heat using the two ensembles. The temperature near the maximum in this larger system is around 2.28, whereas in the 30×30 lattice the temperature near the maximum was 2.30; thus, we see the expected shift in the temperature towards the Onsager value (2.269) for the large system. For the 60×60 lattice at this temperature the microcanonical and canonical specific heats are 2.464 ± 0.02 and 2.226 ± 0.02, respectively. Hence, we see the expected increase in the value of the specific heat as well as the narrowing of the difference of the specific heats in the two ensembles for the larger system; from 0.30 or 16% for the 30×30 system to 0.24 or 10% for the 60×60 system.

In Fig. 4 we show the average of the absolute value of the magnetization in the canonical and microcanonical ensembles, which also shows close agreement between the value of this quantity in the two ensembles. We also calculated the constant energy and constant temperature susceptibilities in the simulations but we have not presented the values of these quantities in this paper. Part of the reason for this is the difficulty of calculating the average value of M in the finite Ising model in zero magnetic fields at temperatures below the transition temperature where in the finite system the lattice spins may turn over while in the thermodynamic limit (Onsager solution) the symmetry is broken; i.e., there is spontaneous magnetization below the transition temperature. In simulations at $T=2.1$ the lattice turns over once in several million moves, which leads to large uncertainties in the value of the magnetization. This problem does not occur for the average of the energy U, the specific heat,

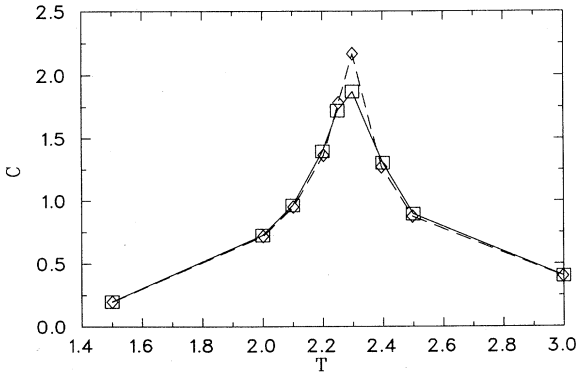

FIG. 2. Configuration specific heat for the nine simulations $c=C/Nk_B$. The solid line and the squares are the canonical ensemble values and the diamonds and dashed line are the microcanonical ensemble values. The lines are just to guide the eye.

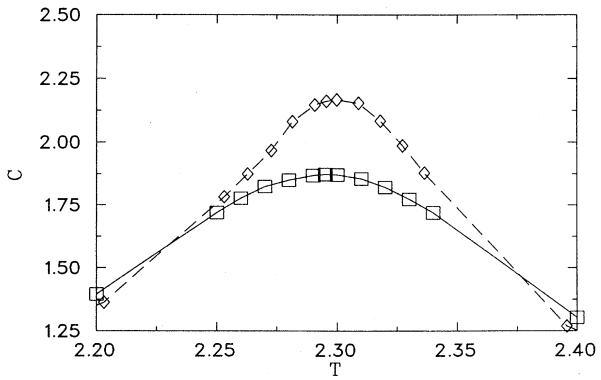

FIG. 3. Region around the maximum in Fig. 2 shown in more detail. The solid line and the squares are the canonical ensemble values and the diamonds and dashed line are the microcanonical ensemble values. The lines are just to guide the eye.

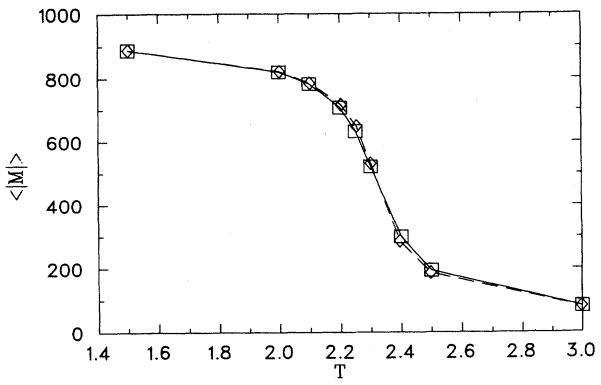

FIG. 4. The average of the absolute value of the magnetization for the nine different temperatures. The solid line and the squares are the canonical ensemble values and the diamonds and dashed line are the microcanonical ensemble values. The lines are just to guide the eye.

or of the absolute value of the magnetization.

The uncertainties or errors estimates we have quoted were determined by making five independent 1×10^6 move runs and finding the standard deviation of the five numbers. In Table I we give the values used to construct Figs 1, 2, and 4 for the canonical ensemble, whereas in Table II we give the microcanonical ensemble values; the error estimates are also included in the tables.

IV. CONCLUSIONS

We have demonstrated that the microcanonical ensemble discussed for continuous potentials in Ref. [2] can also be applied to describe discrete systems and, of course, for continuous and discrete systems. Since the microcanonical ensemble represents an isolated system we feel that this description of a system is at least as fundamental as the canonical ensemble. There is a historical bias against using the microcanonical ensemble because of its complicated form for analytic work; however, in Monte Carlo simulations there is no difference in complexity between the two ensembles and one may use either ensemble: in the canonical ensemble we fix the temperature and determine the energy by an average, while in the microcanonical ensemble we fix the energy and determine the temperature by an average.

We have shown that the ensemble dependence of the specific heat can be easily detected (16%) for a system with 900 spins (10%) for a system with 3600 spins in the vicinity of the maximum of the specific heat. This difference is a precursor to the phase transformation in the Onsager solution. It is possible that this large difference in the values between the same quantity calculated in different ensembles could be used to scan the phase diagram of a system for phase transformations.

For continuous potentials one can generate the microcanonical ensemble by either molecular dynamics or the microcanonical Monte Carlo method. However, for a discrete system only the Monte Carlo method can be used to generate the microcanonical ensemble. One might consider the microcanonical ensemble the more fundamental description of a system since it does not require the introduction of a heat reservoir, but regardless of how one feels about such philosophical statements it is important to know that the microcanonical ensemble is available for use in simulations of discrete systems and can be used to calculate any property that can be calculated in the canonical ensemble. The microcanonical ensemble may be an important tool for unlocking the thermodynamic phase diagram for the system.

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