Microcanonical determination of the order parameter critical exponent

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A highly efficient Monte Carlo method for the calculation of the density of states of classical spin systems is presented. As an application, we investigate the density of states $Ω_N(E, M)$ of two- and three-dimensional Ising models with $N$ spins as a function of energy $E$ and magnetization $M$. For a fixed energy lower than a critical value $E_{c,N}$ the density of states exhibits two sharp maxima at $M = \pm M_{sp}(E)$ which define the microcanonical spontaneous magnetization. An analysis of the form $M_{sp}(E) \propto (E_{c,\infty} - E)^{\beta}$ yields very good results for the critical exponent $\beta_c$, thus demonstrating that critical exponents can be determined by analysing directly the density of states of finite systems.

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I. INTRODUCTION

Substantial progress has been achieved in the understanding of discontinuous phase transitions since the problem has been formulated in microcanonical terms. Till now the microcanonical analysis of continuous phase transitions has only been partly successful. On the one hand it is a great accomplishment that the typical features of symmetry breaking, i.e. the abrupt onset of the order parameter as the critical point is approached from above and the diverging susceptibilities, turn up already for finite systems. This is in contrast to the canonical ensemble where singularities appear exclusively in the thermodynamic limit. On the other hand it is an intriguing and disappointing fact that mean field values have been found for all critical exponents and for all finite system sizes when directly analysing the density of states.

We do not contest the earlier analysis where values of the critical exponents of an Ising system were determined from the expansion of the entropy $S_N(E, M)$ in the vicinity of the critical point of the finite system, situated at $E = E_{N,c}$ and $M = 0$. Here it is our aim to show that the non classical infinite lattice exponents can be obtained directly from the density of states if the expansion of the finite system entropy $S_N(E, M)$ is carried out at the critical point $E = E_{c,\infty}$ and $M = 0$ of the infinite system. (The critical point of the finite or infinite system is defined as the value of the energy $E = E_{c,N}$, where the second derivative $[\partial^2 S_N / \partial M^2]_E$ of the entropy taken at $M = 0$ changes its sign.)

For the purpose of determining the density of states $Ω_N(E, M) = \exp S_N(E, M)$ (in units where $k_B = 1$) we have developed a highly efficient algorithm which is based upon the Broad Histogram method. It allows a precise and speedy determination of the density of states as a function of one, two or even more parameters should it be necessary. In the course of these calculations it will be demonstrated that very good values for the order parameter critical exponent can be obtained by a microcanonical analysis already for relatively small system sizes.

The paper is organized in the following way. In the next Section we present the numerical method which permits us to compute the density of states of classical spin systems with very high accuracy. Section III is devoted to the analysis of the microcanonically defined spontaneous magnetization and to the determination of the corresponding critical exponent. A short summary concludes the paper.

II. NUMERICAL METHOD

One of the aims of computer simulations in statistical mechanics is the determination of averages of observables $X$ of the many particle system under study:

$$\langle \hat{X} \rangle_{\hat{W}} = \sum_{\mu \in \Gamma_\mu} \hat{W}(\mu) \hat{X}(\mu). \quad (1)$$

The space $\Gamma_\mu$ contains an enormous number $\Lambda_\mu$ of microstates and the sum in (1) runs over all of them. $\hat{W}(\mu)$ is a probability distribution on that space and $\hat{X}(\mu)$ is the value of $X$ in the microstate $\mu$.

In all cases of interest $\hat{W}(\mu)$ and $\hat{X}(\mu)$ depend on $\mu$ only via a few parameters $\underline{P} = (P_a, P_b, ...)$, i.e.,

$$\hat{W}(\mu) = W(\underline{P}(\mu)) \quad (2)$$

and

$$\hat{X}(\mu) = X(\underline{P}(\mu)). \quad (3)$$

Examples for $\underline{P}$ might be the interaction energy $E$ of a magnetic system and its magnetization $M$. An example for $W(\underline{P})$ could be the canonical distribution

$$W(E, M) = \frac{\exp [-\beta (E - h M)]}{\sum_{E',M'} \exp [-\beta (E' - h M')]} \quad (4)$$

The parameters $\underline{P}$ characterize the macrostate of the system and examples for $X(\underline{P})$ might be the parameters themselves, their fluctuations as e.g. $(E - <E>_\omega)^2$ or any other function of them.
The unwieldy sum in (4) is greatly reduced if the degeneracies $\Omega(P)$ of the macrostates which are characterized by the parameters $P$ are known. Then:

$$\langle \hat{X} \rangle_W = \langle X \rangle_W = \sum P \Omega(P) W(P) X(P). \quad (5)$$

$\Omega(P)$ is also called the density of states DOS. The number of terms in the sum (4) is already gigantesque for a system of only a few hundred particles: $A_N$ is of order $f^N$ where $N$ is the number of particles in the system. $f$ is equal to 2 for an Ising system and for a $q$-states Potts model $f = q$.

Compared to that, the sum in (3) can be performed with very little effort indeed. Its number of terms is only of order $N^\nu$ where $\nu$ is the number of parameters. Once $\Omega(P)$ is known, the sum in (3) can be performed in the twinkle of an eye by any desktop computer.

Now the difficulty of calculating averages of $X$ has been shifted to the determination of the DOS. This does not seem to be any easier, but we have developed a new algorithm to construct $\Omega(P)$. Before the algorithm is explained in detail we want to point at yet another advantage which is offered at no extra cost when the density of states $\Omega(E,M)$ has been determined. As $\ln \Omega(E,M) = S(E,M)$ (setting $k_B = 1$) is the entropy as a function of its natural variables, the thermodynamic relations can be derived directly from $S(E,M)$ by differentiation. One thereby obtains the microcanonically defined temperature, specific heat, susceptibilities etc.

This is an extra benefit on top of the possibility of having the mean values of any function $X(P)$ (e.g. $X(E,M)$) and for any desired probability distribution $W(P)$ at hand.

The algorithm is a variant of the transition variable method (6). Its starting point is an extremely simple observation: Consider any mechanism which generates a new microstate $\mu'$ when it is applied on the microstate $\mu$. An example for such a mechanism could be a single spin flip in an Ising system. When the single spin flip mechanism is applied to all the $N$ spins of all the $\Omega(P)$ microstates which belong to the macrostate which is characterized by $P$, then $N \Omega(P)$ new microstates are created. Let $V_{ij}$ be the number of them which belong to the macrostate characterized by $P$. As any spin flip can be reversed: $V_{ji} = V_{ij}$. In other words there are as many connections (by single spin flip) from level $P_i$ to level $P_j$ as there are connections from level $P_j$ to level $P_i$. Thus if one chooses one microstate of level $P_i$ at random, selects one spin at random, and flips it, the probability of arriving at level $P_j$ will be $V_{ij}/(N \Omega(P_i))$ and vice versa if we choose one of the spins in one of the states of level $P_j$, at random and apply the mechanism to it, then the probability of arriving at level $P_i$ is $V_{ij}/(N \Omega(P_j))$.

This simple observation is used to create an algorithm which serves two purposes:

i) It determines the rate of attempts $T_{ij} = V_{ij}/(N \Omega(P))$ to go from a starting level $P_i$ to another level $P_j$ which can be reached by the chosen mechanism.

ii) It leads to an equal probability of visiting the levels irrespective of their degeneracy.

Once the $T_{ij}$ have been found it is an easy matter to construct the whole surface $\Omega(P)$ from the ratios $T_{ij}/T_{ji} = \Omega(P_i)/\Omega(P_j)$. In order to calculate the $T_{ij}$ one writes down the total number $Z_i$ of applications of the mechanism while in level $P_i$, and also the number of applications $Z_{ij}$ which would lead to level $P_j$, and this in both cases, if the step is executed or not. Then $T_{ij} = Z_{ij}/Z_i$.

As a reversible transition mechanism we choose single spin flips. Before the spin is flipped the system is characterized by the parameter values $P_i$. A spin is chosen at random. Its flip would lead to a new state characterized by $P_j$. We add 1 to $Z_i$ and also to $Z_{ij}$ whether the flip is accepted or not. After a large number of attempted spin flips $Z_{ij}/Z_i$ approaches $T_{ij}$. The demand ii) is fulfilled, if steps from $i$ to $j$ and from $j$ to $i$ are executed with the same frequency. This can be achieved by introducing probabilities for the acceptance of executing a step. This probability of accepting the step from $i$ to $j$ is equal to 1 if $T_{ij} < T_{ji}$ and it is $T_{ji}/T_{ij}$ otherwise. This equalizes the probabilities

$$p(P_i, P_j + \Delta P) = p(P_j + \Delta P, P_i) \quad (6)$$

of going from a level $P_i$ to the level $P_j + \Delta P$ and of the reverse transition.

Choosing nonzero, but otherwise arbitrary values for $Z_i$ and $Z_{ij}$ for all $i$ and $j$ and starting from any one of the states of the system one rapidly builds up good estimates for the transition rates $T_{ij}$. When this point is reached all levels $P_i$ are visited with the same frequency and the quality of the transition variables is improved with the same rate over the whole parameter range.

The procedure adopted here differs from other implementations of the transition variable method in several respects: The transition variables are updated at every single spin flip, in return we do not register all the possible transitions which are possible from a given microstate, but only those ones which are attempted by the algorithm, whether they are successful or not. Furthermore the transition probabilities $T_{ij}$ are updated during the whole run and the acceptance rates are governed by the most recent value of $T_{ij}$ from the beginning of the simulation to its very end.

This method gives us the freedom of restricting the calculations to a chosen number of channels in energy or magnetization direction. Whereas for not too large systems all values of the energy and of the magnetization may be allowed in a single run, for larger system sizes narrow bands in energy direction covering all magnetization channels may be used. In the limit of only one energy channel per band our approach differs from the well-known Q2R method (7) as for a fixed energy value all the possible magnetizations are visited with the same frequency.
Our algorithm has been subjected to several stringent tests. We have calculated $\Omega_N(E)$ for a $32 \times 32$ Ising model and we have compared the resulting entropy with the exact data of Beale. $S_N(E)$ as well as its first and second derivative match the exact values almost perfectly. For example, $7 \times 10^5$ Monte Carlo sweeps yield for the inverse microcanonical temperature $S_N'(E)$ an average error as small as 0.025% when compared to the first derivative of the Beale data. In a plot of the specific heat $c(E) = -(S_N''(E))/S_N'(E)$ versus temperature $T(E)$, where $1/T(E) = \beta(E) = S_N'(E)$, one cannot distinguish the simulated data from the exact result. For the same system we have also calculated $\Omega_N(E, M)$ from which we again find $\Omega_N(E)$, now by summation over $M$. In addition we find $\Omega_N(M)$ by summation over $E$ and there is excellent agreement with the exact result which is $N!/[N^2 + M^2 N^2 - M^2]$. The algorithm compares very favorably to other methods proposed for the computation of the density of states. Its efficiency for the $32 \times 32$ Ising model is slightly better than that of the multiple-range random walk algorithm of Wang and Landau, where an average error of 0.035% was obtained for $7 \times 10^5$ Monte Carlo updates. It must be stressed that our method is completely different to the Wang/Landau method where a rough estimator of the DOS is built up rapidly due to a multiplicative update of $\Omega(E)$ every time the energy level $E$ is visited. The error introduced by this multiplicative update has to be eliminated before obtaining the DOS with high precision. In our present approach, no such error is introduced during the course of the simulation.

As we will show in the following, the new method enables us to compute the density of states with a high accuracy even for large Ising systems. Furthermore, preliminary results for complex systems with a rough energy landscape are very promising.

As a first application, we compute in the next Section the microcanonical order parameter in the two- and three-dimensional Ising models. It must be noted that data of extremely high accuracy, rarely needed in a canonical study, are mandatory for a reliable determination of microcanonically defined quantities.

### III. MICROCANONICALLY DEFINED SPONTANEOUS MAGNETIZATION

In a microcanonical analysis of finite systems with $N = L^d$ spins ($d$ being the number of space dimensions), the object of interest is the density of states $\Omega_N(E, M)$ as a function of the energy $E$ and the magnetization $M$. We define the spontaneous magnetization $M_{sp, N}(E)$ as the value of $M$ where the entropy $S_N(E, M) = \log \Omega_N(E, M)$ at a fixed value of the energy has its maximum with respect to $M$. At energies lower than a critical value $E_{c,N}$ the entropy exhibits two maxima at $M = \pm M_{sp, N}$. On approach to this point $E_{c,N}$ the order parameter $M_{sp, N}$ vanishes with a square root behaviour in the finite system.

In order to achieve very good statistics we have restricted the calculations to a narrow band which covers only five channels in energy direction, but stretches over all possible values of the magnetization. All single spin flips within this band are allowed. Spin flips which would end up outside the band are rejected. We build up the $T_{ij}$ and from them construct the DOS in magnetization direction. A single flip leads from a microstate in the level $P_j = (E_j, M_j)$ with entropy $S_N(E_j, M_j)$ to a state of a neighbouring level $P_{ij} = (E_i, M_j)$ with $E_{ij} = E_j + 4 \eta$ and $M_j = M_i + 2 \gamma$. Here $\gamma = \pm 1$, whereas $\eta = 0, \pm 1, \pm 2$ for a two-dimensional square lattice and $\eta = 0, \pm 1, \pm 2, \pm 3$ for a three-dimensional simple cubic lattice. The entropy at the macro state at $P_{ij}$ can then be expressed as:

$$S_N(E_j, M_j) = S_N(E_i, M_i) + \beta(E_i, M_i) 4 \eta + \mu(E_i, M_i) 2 \gamma + \ldots$$

where $\beta(E, M) = \partial S_N(E, M)/\partial E$ is the inverse temperature and $\mu(E, M) = \partial S_N(E, M)/\partial M$. Because of the densely spaced energy and magnetization levels (on the intensive scale) higher order terms in $[\Theta]$ may safely be neglected. From ratio of one transition observable pair $T_{ij}/T_{ji} = \Omega(P_j)/\Omega(P_i) = \exp[4\eta \beta + 2 \gamma \mu]$ follows one linear combination of $\beta$ and $\mu$. In two dimensions, the ten states at the magnetizations $M = 1$ and $E_0 + 4 \eta$ within the band of states to which the calculation was restricted, are connected by 12 transition variable pairs. Averaging over the 12 equations which determine $\beta$ and $\mu$ considerably increases the statistical relevance of the data. In three dimensions, the number of transition variable pairs is even larger.

Thus, the transition variable method directly provides the derivative $\beta(E, M)$ of the entropy which we need for the determination of its maximum.

From the zeros of $\mu(E, M)$ the spontaneous magnetization is determined with high precision as shown in Figure 1. The variation of the spontaneous magnetization per spin, $m_{sp, N} = M_{sp, N}/N$, as a function of the specific energy, $\varepsilon = E/N$, is displayed in Figure 2 for two-dimensional Ising models on an infinite and on a small square lattice with $32^2$ spins. The curve for the infinite lattice has been drawn from the exact results for $E(T)$ and $E(T)$.$^{[6]}$ Both curves coincide at low energies. In our analysis, $M_{sp}(E)$ for energies lower than the critical value $E_{c, \infty}$ of the infinite system is fitted by

$$M_{sp}(E) = A|\varepsilon^*|^{\beta_{c, eff}(E)}$$

with an energy dependent effective exponent $\beta_{c, eff}(E)$. Here, $\varepsilon^* = (E_{c, \infty} - E)/(E_{c, \infty} - E_g)$ is the reduced energy. $E_g$ denotes the ground state energy. The effective exponent, which is given by $\beta_{c, eff} = d\ln M_{sp}/d\ln |\varepsilon^*|$, yields the critical exponent $\beta_\varepsilon$ in the limit $E \rightarrow E_{c, \infty}$. Contrary to Ref.$^1$, the critical expansion refers to $E_{c, \infty}$. 


and not to the critical energy of the finite system. The procedure has been performed for a series of system sizes $N_1 < N_2 < N_3 \ldots$ In the energy range where $N_i$ and $N_{i+1}$ yield the same exponent $\beta_{\varepsilon,\text{eff}}(E)$ this exponent is selected for the plot in Figure 3. This value of $\beta_{\varepsilon,\text{eff}}(E)$ is used up to the energy where the two exponents start to differ from each other, i.e. until finite size effects show up. Then we plot the common exponent for the system sizes $N_{i+1}$ and $N_{i+2}$ until these begin to disagree and so on. The largest systems for which we have performed these calculations were $700 \times 700$ in two dimensions and $80 \times 80 \times 80$ in three (these are presumably the largest Ising systems for which microcanonical quantities have ever been determined). This approach has the advantage that the finite-size effects are monitored closely. Furthermore, one avoids to simulate unnecessarily large systems at low energy where small systems already yield data essentially free of finite-size effects.

The critical exponent $\beta_\varepsilon$ is related to the commonly used exponent $\beta$ which describes the behavior of the order parameter with respect to the temperature by $\beta_\varepsilon = \beta/(1 - \alpha)$ where $\alpha$ is the usual specific heat critical exponent. In two dimensions where $\alpha = 0$ we expect $\beta_\varepsilon = 1/8$, in three dimensions with $\beta = 0.327$ and $\alpha = 0.11$ we expect $\beta_\varepsilon = 0.367$.

Also shown in Figure 3 is the corresponding effective exponent derived from the exact result $M(E)$ of the infinite two-dimensional Ising model. Obviously, the numerical data follow closely the exact result, thus demonstrating the reliability of our algorithm for computing accurate microcanonical quantities even for large systems.

Figure 3 exhibits two peculiarities of the 2D system: (i) The strong $N$ dependence of $E_{c,N}$ makes it extremely difficult to obtain data points for $|\varepsilon^*| < 0.2$. (ii) The effective critical exponent $\alpha_{\varepsilon,\text{eff}}(t)$ of the specific heat $c(t)$ of the infinite system is finite for finite $t = (T_c - T)/T_c$, but precipitates to zero as $t = 0$ is approached. This
causes the dramatic behavior of $\beta_{\varepsilon,\text{eff}}(\varepsilon^*) = \beta_{\text{eff}}/(1 - \alpha_{\text{eff}})$ in the vicinity of $|\varepsilon^*| = 0$.

Remarkably, good values of the exponents are already found for the smallest systems considered here, namely $L = 50$ in two and $L = 10$ in three dimensions. This is especially true for the three-dimensional case where, over the whole energy range considered, the value of the effective exponent does not noticeably differ from the value of the critical exponent. Even for energies more than 30% below the critical energy and for systems consisting of only 1000 spins, the obtained effective exponent is almost identical to the critical exponent. This is in marked contrast to a similar canonical analysis of the behaviour of the order parameter with respect to the temperature where large corrections to scaling lead to an effective temperature dependent exponent which differs by almost 50% from the value of the critical exponent at temperatures some 30% below $T_c$.

The origin of the different behaviour of $\beta_{\varepsilon,\text{eff}}$ as function of the reduced energy in two and three dimensions can be traced back to the logarithmic divergence of the specific heat in the two-dimensional Ising model. We expect a behaviour similar to that observed in the three-dimensional Ising model for all models with a non-vanishing specific heat critical exponent. Future investigations of various models will be needed to clarify this point.

**IV. SUMMARY**

We have developed an algorithm which rapidly builds up transition variables for any reversible rule of jumping from one macrostate of a system, characterized by a set $\mathcal{P}$ of parameters, to another one. The most recent values of the transition variables govern the further path of the system through phase space in such a way that equally good statistics is obtained over the whole area which is covered by the calculation. As an example we have chosen the two- and three-dimensional Ising models with $\mathcal{P} = (E, M)$ together with single spin flips as the transition mechanism. From the transition observables we obtain highly accurate data for $dS/dM$ which allow a precise determination of the microcanonically defined spontaneous magnetization $M_{sp}(E)$. An analysis of $M_{sp}(E)$ for different system sizes yields excellent values for the order parameter critical exponent $\beta_c$. 

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