First order phase transitions studied in the dynamical ensemble

The $q$-states Potts model as a test case

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Abstract. A knowledge of the density of states $\Omega(\varepsilon)$ of a many particle system ($\varepsilon$ is the energy per particle) contains the complete information about its thermal behaviour. In this paper it will be demonstrated that $\Omega(\varepsilon)$ can very efficiently and precisely be determined by a Monte Carlo calculation in an ensemble where the system of interest is coupled to another system of comparable size. This is in contrast to the canonical approach where the system of interest is coupled to an infinite bath at a temperature $T$. The usefulness of the approach will be demonstrated for the $q$-states Potts model with $q = 4, 5, \text{ and } 8$ where the numerical data can be compared with exact results. In our numerical data we can clearly identify a first order phase transition for $q \geq 5$ and a second order transition for $q = 4$.

I. Introduction

Over many years numerical data on continuous and discontinuous phase transitions have been gathered using Monte Carlo methods in the canonical ensemble. Very efficient algorithms have been developed and recently the original Metropolis [1] sampling method has been replaced by powerful cluster methods as e.g. the Swendsen-Wang [2] or the Wolf [3] algorithm.

The $q$-states Potts model [4] with the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} + 2N \varepsilon$$ \hspace{1cm} (1)

and nearest neighbour interactions on a two-dimensional square lattice, is frequently chosen as a testing ground for numerical calculations [5-7] because its properties at the transition are known exactly. Baxter [8] has shown that the transition is continuous for $q \leq 4$ and discontinuous for $q > 4$, he has also calculated the exact values of the transition temperature $T_0$ and for $q > 4$ the energies $\varepsilon_1$ and $\varepsilon_u$ at the lower and upper limits of the two-phase region.

For large values of $q$ the transition is strongly first order and there is no problem in interpreting the numerical data. Binder [9] cautions that care is needed in the analysis of Monte Carlo data of the Potts model already for $q = 8$, and that for $q = 5, 6$ even the qualitative distinction of the first-order character of the transition is difficult.

Rarely has a heat bath other than the infinite canonical one been used in an MC-calculations. Notable exceptions are the Creutz demon [10], a small system that exchanges energy with the spins of an Ising system, and the Gaussian bath introduced by Challa and Hetherington [11]. The latter is a finite bath (with a Gaussian density of states) which is in contact with the system of interest.

In the following it will be demonstrated that with an appropriately chosen finite bath one can very accurately determine the transition temperature $T_0$ as well as $\varepsilon_1$ and $\varepsilon_u$. For $q = 8$ high precision is obtained with little exercise, whereas a moderate effort is needed for $q = 5$. The difference between the discontinuous transition at $q = 5$ and the continuous one at $q = 4$ is clearly exhibited.

In its main point this paper goes beyond the goals of [11] and beyond the application to the Potts model. It will be shown, how one can retrieve $\Omega(\varepsilon)$, the density of states of the system of interest, from the numerical data. $\Omega(\varepsilon)$ is the most valuable information available about the system. A finite bath of kinetic energy (ideal gas) turns out to be very expedient for our purpose.

II. The dynamical ensemble

The approach in this paper is motivated by a recent molecular dynamics calculation [12, 13] of the phase transition in the modified $xy$ model. There the configurational energy $E$ of the rotors is a continuous function of angles. If the kinetic energy $K$ of the rotors is added to $E$ one obtains the total Hamiltonian $G = E + K$. $E$ and $K$ are coupled in a natural way by Hamilton's equations of motion. The total energy $G = E + K$ is a constant...
of the motion, but there is a permanent exchange of energy between the two parts of the combined system as it passes through its equilibrium states.

Here we are interested in the thermal behaviour of a discrete $N$-particle system $\mathcal{K}_N$, the $q$-states Potts model, with no compelling way of implementing dynamical equations. Again its thermal behaviour is completely determined by its density of states

$$\Omega_N(\varepsilon) = \exp \left\{ N s_N(\varepsilon) \right\}. \quad (2)$$

Here $\varepsilon = E/N$ is the energy per particle and $s_N(\varepsilon)$ the microcanonically defined entropy per particle. It is the aim of this paper to establish $s_N(\varepsilon)$ as precisely as possible from MC-data.

To this end the Monte Carlo method will be modified in such a way that an exchange of energy occurs between the $N$-particle Potts-system $\mathcal{K}_N$ and a finite reservoir $\mathcal{K}_M$ which in our case is an ideal gas with $M$ degrees of freedom and kinetic energy $K$. The density of states of $\mathcal{K}_M$ is known. We then study the microcanonical ensemble at the temperature $T = \frac{2}{\beta}$ and the probability distribution $P_G$ develops into the canonical distribution $\frac{1}{Z} e^{-\beta G}$. An appropriate form for $\frac{1}{Z} e^{-\beta G}$ can be viewed as an effective inverse temperature $\beta = \frac{1}{k_B}$ where $k_B = \frac{J}{N}$. These temperatures are related by $\beta = \frac{1}{k_B}$.

Some of the advantages of such an approach have already been demonstrated by Challa and Hetherington [11]. There it was a system with large values of $N$ because (10) is correct within a factor $(1 - \xi)$ where $\xi = \frac{2}{N} \frac{[\xi(\varepsilon_b - \varepsilon_a)]^2}{N - 2}$ is of order $1/N$. The MC-method is then performed in the same manner as in the canonical ensemble.

The only difference is a dynamical adjustment of the effective inverse temperature $\xi$ during a run. Since the energy of $\mathcal{K}_N$ is monitored anyway, this does not require further numerical effort.

In a run at constant $G$ the energy per particle $\varepsilon$ is sampled and the mean value $\langle \varepsilon \rangle_G$ is formed over many sweeps through the lattice. Then $\langle k \rangle_G$ is equal to $\langle k \rangle_G = \frac{G}{N} \langle \varepsilon \rangle_G$ and $\langle \varepsilon \rangle_G$ is plotted versus $2 \langle k \rangle_G$. In Fig. 1 these data are shown for $q = 8, 5, 4$ and $3$ and for several lattice sizes $N = L \times L$. The data of Fig. 1 are analyzed in terms of a density of states $\Omega_N(\varepsilon) = \exp \left\{ N s_N(\varepsilon) \right\}$. An appropriate form for $s_N(\varepsilon)$ (see (13), containing a set of adjustable parameters, is inserted into (5) and (6) and the parameters are determined by a least squares fit of $\langle \varepsilon \rangle_G$ as a function of $2 \langle k \rangle_G$. The optimal fits are shown as full lines in Fig. 1.

The resulting expression for $s_N(\varepsilon)$ can be used to directly plot the microcanonically defined temperature $T_N(\varepsilon) = \frac{1}{\beta_N(\varepsilon)}$ (with $\beta_N(\varepsilon) = \frac{d s_N(\varepsilon)}{d \varepsilon}$) as a function of $\varepsilon$. This is shown in Fig. 2 (with coordinate axes interchanged).

There are two very important points to be made here:

(i) There is only little difference between the two sets of curves in Figs. 1 and 2. For $L = 64$ these differences become almost invisible. This means that our data do establish $T_N(\varepsilon)$ (as a function of $\varepsilon$ in Fig. 2) with the same precision as they allow the determination of $2 \langle k \rangle_G$ as a function of $\langle \varepsilon \rangle_G$ (in Fig. 1). The dynamical ensemble thus provides a direct and stringent access to $T_N(\varepsilon)$, i.e. to $\beta_N(\varepsilon)$ and $s_N(\varepsilon)$ or the density of states.

The microcanonical ensemble of systems $\mathcal{K}_{NM}$ (i.e. $M = N$) at constant total energy $G$ will be called the dynamical ensemble for $\mathcal{K}_N$. This name is chosen because the ensemble is very naturally realized in a MD-simulation as has been demonstrated for the modified $q \times q$ model in [12].

In order to find the appropriate transition probabilities, we compare with a conventional Metropolis MC-calculation with coupling to an infinite bath. There the canonical distribution

$$p_T(\varepsilon) = \varepsilon^{N s_N(\varepsilon)} e^{-N \beta \varepsilon} \quad (7)$$

is generated by choosing the transition probabilities $w_{\varepsilon \rightarrow \varepsilon^\prime}$ between two states $\varepsilon$ and $\varepsilon^\prime$, such that the detailed balance at the bath temperature $T = 1/\beta$ is fulfilled:

$$w_{\varepsilon \rightarrow \varepsilon^\prime} w_{\varepsilon^\prime \rightarrow \varepsilon} = e^{-\beta \varepsilon^\prime} e^{-\beta \varepsilon} \quad (8)$$

where $E_a = N \varepsilon_a$ and $E_b = N \varepsilon_b$ are the energies of the system $\mathcal{K}_N$ in the two states $a$ and $b$, respectively.

Correspondingly in the dynamical ensemble (with $M = N$) where the distribution of (5) must be realized, the transition probabilities have to meet the condition:

$$w_{\varepsilon \rightarrow \varepsilon^\prime} w_{\varepsilon^\prime \rightarrow \varepsilon} = \frac{\varepsilon^\prime}{\varepsilon} e^{-\beta \varepsilon^\prime} e^{-\beta \varepsilon} \quad (9)$$

During a MC-run spin flips are accepted or rejected in such a way that (9) is fulfilled. For reasons of numerical convenience this ratio is approximated by:

$$w_{\varepsilon \rightarrow \varepsilon^\prime} w_{\varepsilon^\prime \rightarrow \varepsilon} = e^{-\xi(N_b - N_a)}, \quad (10)$$

where $\xi = \frac{2}{N} \frac{[\xi(\varepsilon_b - \varepsilon_a)]^2}{N - 2}$ is of order $1/N$. The MC-calculation in the dynamical ensemble is then performed in the same manner as in the canonical ensemble. The only difference is a dynamical adjustment of the effective inverse temperature $\xi$ during a run. Since the energy of $\mathcal{K}_N$ is monitored anyway, this does not require further numerical effort.

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