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Microcanonical simulations with a large number of demons

Christophe Dress

Laboratoire de Physique Théorique†, ENS 24, rue Lhomond, F-75231 Paris Cedex 05, France

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Abstract. We generalize the microcanonical algorithm developed by Creutz *et al*, and make a detailed comparison with the exact solution in the case of a two-dimensional Ising model at finite volume. We present a new numerical method to compute the temperature in the microcanonical ensemble. This allows us to define a 'thermalization' criterion to estimate the point where the differences between canonical and microcanonical results are the smallest. This criterion is shown to work well in the case of the two-dimensional Ising system.

1. Introduction

Monte Carlo (MC) simulations have become a classical tool with which to investigate a large number of problems in physics [1]. Since the first MC algorithm of Metropolis *et al* [2], there has been an ongoing quest for faster algorithms, either to beat critical slowing down or to cope with intrinsically slow dynamics such as aging effects in glasses or in disordered systems. Microcanonical algorithms, first proposed by Creutz [3], are typical examples of such algorithms.

The principle of the microcanonical algorithms developed by Creutz *et al* is as follows. One adds to the physical system under study a set of uncoupled discrete and bounded energy reservoirs, historically called demons. A new configuration of the whole system, formed by the physical system and the demons, is produced by flipping a spin, and simultaneously changing the energy of one demon in such a way that the total energy is conserved. This new configuration is accepted each time the energy difference of the physical system can be absorbed by the energy reservoir of the demon (see section 2 for a detailed description of the algorithm). This algorithm is deterministic and can be implemented using only Boolean operations and multispin coding. This is the reason it is fast. For two-dimensional Ising models, and, when the number of demons is fixed or small compared to the number of spins, this microcanonical algorithm has been studied by Creutz *et al* [4–6] and in the context of finite-size scaling by Desai *et al* [7]. More recently Creutz has also shown how to combine microcanonical dynamics with cluster algorithms [8].

A significant difference between canonical and microcanonical algorithms is that in the former case the temperature is an input but the energy has to be computed during the simulation while in the microcanonical case the energy is the input and the temperature has to be computed. Creutz made the hypothesis that the demon energies obey the Boltzmann distribution (this hypothesis can be checked numerically) and computed the temperature from it. We propose in this paper a new way of computing the temperature, using the Dobrushing–Lanford–Ruelle equations (see later). To compare the microcanonical simulations with the canonical results, one invokes the ensemble equivalence in the thermodynamic limit. Of

† Unité propre du CNRS, associée à l'Ecole Normale Supérieure et à l'Université de Paris Sud.

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course this equivalence is not exact in the simulations because of finite-size effects. In this paper, we make a detailed study of these finite-size effects and their volume dependence in the case of a two-dimensional Ising model. We consider a family of microcanonical algorithms, each algorithm differing in the number of demons (see later; we take nN demons, where N is the number of spins and $n = 1, 2, \ldots, 16$). We simulate the two-dimensional Ising model using this family of microcanonical algorithms and compute the difference from the exact solution in the canonical ensemble which is known for any finite size [9]. We show that these differences go to zero when the volume N or when the ratio n defined above as the number of demons over the number of spins, goes to infinity. We also propose a 'thermalization' criterion, also valid in the cases where we do not have an exact solution, to estimate when these differences are small. Let us call β_{Cr} the inverse value of the temperature computed in the microcanonical ensemble using the Creutz method and β_{DLR} the inverse value of the temperature computed using the Dobrushing–Lanford–Ruelle equations. We propose to take $\beta_{Cr} - \beta_{DLR}$ as an estimator of the difference between the canonical and microcanonical results. We show that this criterion works well in the case of the two-dimensional Ising model.

Originally microcanonical algorithms were proposed because they were faster than the Metropolis algorithm. We would like to stress here another motivation for their study, related to the breaking of ergodicity. One of the major difficulties in the study of disordered systems is the existence of high energy barriers separating local energy minima ('valleys'). For finite volumes the height of the barriers is finite. Any canonical algorithm will jump from one valley to the other, provided one waits long enough, in other words the system is fully ergodic for finite volumes. Ergodicity breaking can only appear in the infinite volume limit. Microcanonical algorithms, on the other hand, display a very different behaviour. The system remains trapped and explores the valley where it was at time zero, providing, of course, there is not enough energy available to jump over the barrier. It may be physically interesting, in certain cases, to average over configurations inside a single valley. This is possible with the microcanonical algorithm [10]. Before applying the microcanonical algorithm to such interesting but difficult cases, we would like to gain a better understanding of it by studying a system over which we have full control. This is the purpose of the present paper. In the case of the existence of a single valley, as in the case of a ferromagnet above the Curie temperature, it has been argued by Bhanot *et al* that the microcanonical algorithm is ergodic provided a small amount of randomness is added, and our simulations confirm this.

This paper is organized as follows. Section 2 contains a presentation of the microcanonical algorithm. In section 3, we present a new method to compute the effective temperature. In section 4, the critical dynamical exponent is evaluated and found to be close to the exponent of the Metropolis algorithm [15, 12]. We discuss the advantages of the different methods to obtain the temperature, propose the criterion defined as above, and investigate other thermodynamical variables, such as the energy fluctuations of microcanonical simulations. The role of the ratio n, the number of demons over number of spins, is investigated and we show that the best results are obtained for a large ratio n. This does not reduce the speed of the simulations. Conclusions are presented in the final section.

2. Microcanonical dynamics

Consider a system denoted by S formed by the union of two independent subsystems. The first subsystem is a ferromagnetic Ising spin system on a two-dimensional square lattice of

finite volume N, with periodic boundary conditions, which we denote by $\mathcal{I}$. The second subsystem is a set of nN independent demons, denoted by $\mathcal{D}$. A demon is characterized by a discrete energy variable e^d, constrained to be between two limit values, $e^d_{\min}$ and $e^d_{\max}$. So the total energy of the whole system is

$$\mathcal{H}_S = \mathcal{H}_\mathcal{I} + \mathcal{H}_\mathcal{D} = -\frac{J}{4}\sum_{\langle ij\rangle} s_i s_j - \sum_{\substack{i=1,\dots,N \\ k=1,\dots,n}} e^d_{i,k}. \tag{2.1}$$

As usual the first sum is over nearest-neighbouring spins in the Ising subsystem, and the coupling constant J is positive. The factor of 1/4 in the Ising energy is chosen so that flipping a spin requires an energy which is a multiple of J. In the following, we will denote by $N(i)$ the set of spins which are the nearest-neighbours of the spin s_i. With this notation the local energy of the spin s_i is defined as $\sum_{j\in N(i)} s_i s_j$.

A microcanonical dynamics which conserves the total energy is imposed on the whole system $\mathcal{S}$. Let us define a single step of this dynamics. An elementary move $m_{i,k}$, formed by flipping the spin s_i and changing the energy of demon indexed by (i,k) to a new value $e'^d_{i,k}$, is called *possible* if the sum of local energy of the spin and the energy of the demon can be maintained unchanged during this move, i.e. if there exists $e'^d_{i,k} \in \{e^d_{\min},\dots,e^d_{\max}\}$ such that the local energy of the spin s_i remains unchanged after the move. If s_i and $e^d_{i,k}$ are the values of the spin and of the demon energy respectively, the new values $s'_i = -s_i$ and $e'^d_{i,k} = e^d_{i,k} + J/2\sum_{j\in N(i)} s_i s_j$, are accepted provided $e^d_{\min} \leqslant e^d_{i,k} \leqslant e^d_{\max}$. In this case, the total energy $\mathcal{H}_\mathcal{S}$ does not change. A single step of the dynamic consists in choosing a spin s_i and a demon indexed by (i,k), and accepting the move $m_{i,k}$, if it is *possible*. In the microcanonical ensemble where the equilibrium distribution is uniform, this dynamics checks the detailed balance, i.e. if the elementary move $m_{i,k}$ is accepted then the inverse move is also accepted as a *possible* move, and with probability one in both cases. No rigorous proof of ergodicity exists, but the introduction of a small amount of randomness should ensure ergodicity, especially since the system can only be trapped by energy barriers which are at least proportional to the number of spins. This problem has been carefully discussed by Bhanot *et al* [4] in the case of a small number of demons compared to the number of spins.

The implementation of the algorithm is now briefly described. A multispin coding algorithm is used with 16 spins for each 32-bit word, allowing updating of 16 spins simultaneously. The capacity of energy storage of each demon $e^d_{\max} - e^d_{\min}$ is fixed to $3J$, and 16 demons are coded in each 32-bit word. All the algebra for updating and measurement needs only Boolean-type or integer-type operations. At the beginning a disordered sequence combining spins and demons, in which n demons are linked preferentially to one single spin, is fixed. After several lattice sweeps, we change randomly this updating order and shuffle the demons, thus introducing randomness which makes the algorithm non-deterministic and prevents experimentally any ergodicity breaking. This small amount of randomness has a negligible effect on the speed of the algorithm.

3. Determination of temperature

To compare the microcanonical simulations with the exact canonical results requires a method to extract the temperature from the simulations.

The first method was presented by Creutz [3] and her principle relies on the fact that, at the thermodynamic limit, the two subsystems $\mathcal{I}$ and $\mathcal{D}$ are 'in equilibrium' at the same temperature. In the canonical ensemble, the partition function of the whole system $\mathcal{S}$

decouples itself into a product of two partition functions, one for the Ising spin subsystem, the other for the demon subsystem. The energy of the demons is then distributed with a Boltzmann law at the temperature $1/\beta$, and the probability $P(e)$ that a demon, randomly chosen, has the energy e is

$$P(e) = \frac{\exp(-\beta e)}{\sum_{[e']} \exp(-\beta e')}. \tag{3.1}$$

This implies the following relation in the canonical ensemble

$$\beta = \frac{1}{e - e'} \log \frac{P(e')}{P(e)}. \tag{3.2}$$

Then, for a large volume N, this relation is checked in the microcanonical simulations by making use of the ensemble equivalence at the thermodynamic limit. If the dynamics is ergodic (experimentally it is so), $P(e)$ can be replaced by the time-averaged fraction of demons possessing the energy e. In these conditions, we can compute the first effective temperature, denoted by β_{Cr}, by taking the average of all the β corresponding to different energy values, and errors bars come naturally from the variance of the data. We will discuss in the next section the quality of the fit by computing the χ^2.

We now propose a new method, using only the spin subsystem $\mathcal{I}$, to extract a temperature from the simulations. This method is based on the Dobrushin–Lanford–Ruelle (DLR) relations [14], valid in the canonical ensemble, which express that a given region is in thermal equilibrium with its surroundings. In the general case where the coupling constants J_{ij} are not identical, for the two-spin correlation function $\langle s_0 s_1 \rangle$, the relation reads

$$\langle s_0 s_1 \rangle - \left\langle \frac{\mathrm{e}^{-\beta J_{01}} \cosh \beta F_+ - \mathrm{e}^{\beta J_{01}} \cosh \beta F_-}{\mathrm{e}^{-\beta J_{01}} \cosh \beta F_+ + \mathrm{e}^{\beta J_{01}} \cosh \beta F_-} \right\rangle = 0 \tag{3.3}$$

where $F_+ = F_0 + F_1$, $F_- = F_0 - F_1$, and $F_0 = \sum_{i \in N(0)} J_{0i} s_i$, $F_1 = \sum_{i \in N(1)} J_{1i} s_i$ being the fields acting respectively on the spins s_0 and s_1. Brackets $\langle \cdots \rangle$ denote an average over all the configurations. Formula (3.3) is only valid in the canonical ensemble. But in the microcanonical ensemble, it also allows us to define an effective temperature as follows. From the simulations, we compute the joint probability $P(F_0, F_1)$ that (F_0, F_1) were the fields acting on the spins s_0, s_1, and the average $\langle s_0 s_1 \rangle$. The second term of the equation (3.3) then becomes a computable function of β and the local temperature sought corresponds to a zero of this equation. The final effective temperature which we will denote by $1/\beta_{\mathrm{DLR}}$ is given by averaging those local temperatures over each couple of neighbouring spins. The ensemble equivalence ensures that, at infinite volume N, this effective temperature coincides with the one imposed on the canonical ensemble.

We would like to stress the following important point: the (DLR) relations are local. This implies that (DLR) relations are also verified in the case where average over configurations is only over a subset of the full set of possible configurations. For example, in a ferromagnet below the Curie temperature these relations are still valid even if the sum is only over configurations of positive magnetization. In particular this means that these relations remain true in each ergodic subsystem, when there is ergodicity breaking. Thus, for spin glasses, they should be true below the transition temperature. This method would then determine a temperature corresponding to the configurations which can be reached inside a single valley.

In the case of a two-dimensional finite-size Ising model, exact expressions for the partition function and other relevant quantities, such as, for example, the energy, have been explicitly given by Ferdinand and Fisher [9]. This result allows a comparison between the effective temperatures $1/\beta$ coming from the simulations and the temperature of the canonical ensemble, corresponding to the energy of the simulation, and takes into account

in a natural way all finite-size effects. We note this temperature β_{FF}. Moreover this exact solution also yields other thermodynamically relevant quantities, such as the heat capacity, which can be fruitfully compared to the microcanonical results.

It is clear that the relation of fluctuation–dissipation for the energy is still not true in the microcanonical ensemble. However, measuring the energy fluctuations constitutes a rather good way to estimate the gap between the distribution we are simulating and a canonical distribution. So let us define the microcanonical energy fluctuations $\tilde{C}$ for the Ising subsystem in our microcanonical ensemble by

$$\tilde{C}_{N,n}(\beta) = N\beta^2[(\mathcal{H}_{\mathcal{I}} - [\mathcal{H}_{\mathcal{I}}]_{\mu c})^2]_{\mu c} \tag{3.4}$$

where the brackets $[\cdots]_{\mu c}$ denote an average in the microcanonical ensemble. Clearly, $\tilde{C}$ depends strongly on the number n of demons per spin, since the conservation of the total energy $\mathcal{H}_S$ leads to the following equality between the energy fluctuations in the two subsystems $\mathcal{I}$ and $\mathcal{D}$: $(\mathcal{H}_{\mathcal{I}} - [\mathcal{H}_{\mathcal{I}}]_{\mu c})^2 = (\mathcal{H}_{\mathcal{D}} - [\mathcal{H}_{\mathcal{D}}]_{\mu c})^2$. Therefore $\tilde{C} = 0$ if there is no demon. For N fixed, and when n is large, we show in appendix A the sketch of the proof that the Ising subsystem distribution tends towards the canonical Boltzmann distribution. *This implies that when n is large, the canonical heat capacity is recovered for $\tilde{C}$.*

4. Results and discussion

The evaluation of the exponential autocorrelation time yields the two major following pieces of information: when it is computed at the critical temperature, it allows one to estimate the critical dynamical exponent; it also enables a rough estimation to be made of the number of steps that must be discarded before taking measurements.

Typically, for an observable B the autocorrelation function $C_B(t)$ decays exponentially:

$$C_B(t) = \frac{\langle B(0)B(t)\rangle - \langle B(0)\rangle^2}{\langle B(0)^2\rangle - \langle B(0)\rangle^2} \approx e^{-t/\tau_{\exp,B}} \tag{4.1}$$

where $\tau_{\exp,B}$ is the exponential autocorrelation time. The dynamical finite-size scaling hypothesis leads to the relation $\tau_{\exp,B}(L) \sim L^{z_B}$, for asymptotically large L and $T = T_c(L = \infty)$. As it is generally believed that for Ising models this dynamical exponent does not depend on the observable B [15, 16], we have chosen to evaluate this exponent z for the energy of the Ising subsystem. In the simulations, the energy which is the input parameter is fixed to the value corresponding to $T_c(\infty)$. Since the evaluation of the integrated autocorrelation time and of the exponential autocorrelation time may lead to different exponents [11], we have computed the exponential autocorrelation time by a fit of the linear part of $\log[C_E(t)]$. Precisely, the autocorrelation function $C_E(t)$ has been approximated by

$$C_j = \frac{1}{D_1 D_2}\left(\frac{1}{M-j}\sum_{i=1}^{M-j} E_i E_{i+j} - \frac{1}{(M-j)^2}\sum_{i=1}^{M-j} E_i \sum_{i=j+1}^{M} E_i\right) \tag{4.2}$$

where M is the length of the time-series for the energy, and

$$\begin{aligned} D_1 &= \left(\frac{1}{M-j}\sum_{i=1}^{M-j} E_i^2 - \frac{1}{(M-j)^2}\left(\sum_{i=1}^{M-j} E_i\right)^2\right)^{1/2} \\ D_2 &= \left(\frac{1}{M-j}\sum_{i=j+1}^{M} E_i^2 - \frac{1}{(M-j)^2}\left(\sum_{i=j+1}^{M} E_i\right)^2\right)^{1/2}. \end{aligned} \tag{4.3}$$

The error bars have been extracted from eight different simulation runs. We show in figure 1, the dependence of $1/\tau_{\exp}$ with the linear size L of the lattice. The critical exponent z is obtained from a least-squares fit of the slopes of the curves $\log(\tau_{\exp,E}) = \text{constant} + z \cdot L$, for two different values of n. For $n = 1$, we found $z = 2.38 \pm 0.27$, and for $n = 8$, $z = 2.09 \pm 0.15$. These results show that the dynamical critical exponent does not seem to depend on the ratio n, and that there is no perceptible difference between this critical exponent and the one deduced from a local algorithm for the two-dimensional Ising system [12]. These results are also compatible with other results [13] obtained from the original version of Creutz's algorithm. This shows that critical slowing down persists in the microcanonical simulations, and this is as expected, since when n is large the algorithm tends towards the Metropolis algorithm.

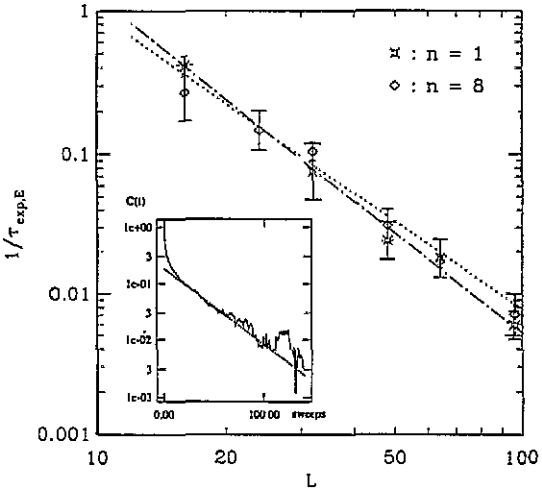

Figure 1. Inverse of the autocorrelation time for the energy $1/\tau_{\exp,E}$ as a function of the linear size of the lattice L, for $T = T_c$, for $n = 1$ and $n = 8$. The dash-dotted curve (— · —) represents the fit for $n = 8$ and the dotted curve (– – –) for $n = 1$. We show in the inset an example of a typical autocorrelation function for $L = 48$ and $n = 8$.

Let us now discuss the demon energy distribution. Let be $N_m(e)$ the number of times that a demon has the energy e in m measurements (therefore $\sum_e N_m(e) = m$). The quality of the fit of $N_m(e)$ by the distribution $mP(e)$ ($P(e)$ is given by the equation (3.1), and $\beta = \beta_{Cr}$), is expressed by $\chi^2 = \sum_e (N_m(e) - mP(e))^2/\sigma(e)^2$, where $\sigma(e)$ is the variance of $N_m(e)$. We have estimated $\sigma(e)$ by dividing the simulation run in 16 blocks and computing the variance of the different $N_{m/16}(e)$. Typically, far from the critical temperature ($|T - T_c| > 0.1$), $\chi^2 \approx 0.04$ for one degree of freedom, for a 64×64 lattice, independently of both the number of measurements, and on the volume N of the Ising system. This means that the hypothesis that demon energy obeys the Boltzmann distribution fits our data very well far from the critical temperature. Further we show in appendix B that if the energy distribution of demons is Boltzmannian, then the microcanonical algorithm is rigorously equivalent to the Metropolis algorithm.

The estimation of the time of the diffusion of the energy through the set of demons constitutes an important measure of the equilibration time of the $\mathcal{D}$ subsystem. Suppose the system is thermalized: we redistribute the demon energy in such a way that the maximum number of them has energy either $e^d_{\max}$ or $e^d_{\min}$, and we resume the dynamics. The energy of the demons is going to diffuse through the whole set of demons. How much time will we

need to again be in a thermalized state? We have estimated this time by computing at each sweep a quantity Q, defined as the squared distance between the rearranged distribution and the Boltzmann distribution at the temperature $1/\beta$:

$$Q = \frac{1}{\mathcal{Z}} \sum_{\{e\}} (N\mathrm{e}^{-\beta e} - N(e))^2 \tag{4.4}$$

where $N(e)$ is defined as the number of demons having energy e, and the normalization $\mathcal{Z} = \sum_{\{e\}} N\mathrm{e}^{-\beta e}$. We plot Q on a logarithmic scale against time in figure 2. Exponential convergence of $N(e)$ towards the Boltzmann distribution is found, with a characteristic time equal to 2.5 lattice sweeps for a 96×96 lattice near $\beta \approx 0.27$. After 20 lattice sweeps we again find fluctuations identical to those when the system is at the thermal equilibrium. Therefore, the energy diffuses very quickly through the set of demons. Let us recall that we permute the demons after each 10th lattice sweep: if we only mix randomly the set of demons every 100 lattice sweeps, the characteristic time is increased by a factor of order 5.

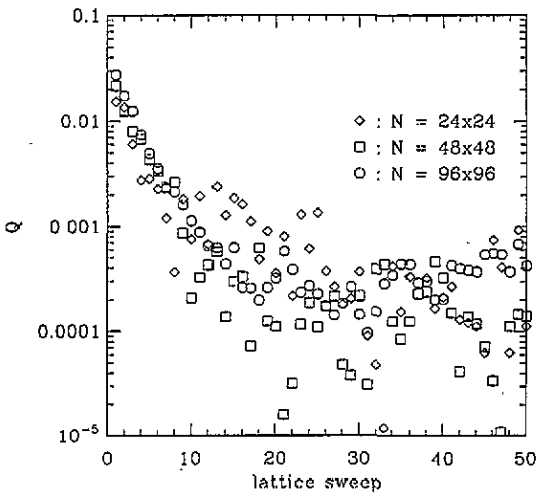

Figure 2. Variation of the quadratic distance Q between the demon distribution and the thermalized distribution of the temperature $1/\beta$ against time counted in lattice sweeps for a temperature around $\beta \approx 0.27$, and for different lattice sizes ($n = 1$).

Moreover, we deduce from our simulations that for lattices of size lesser or equal to $L = 128$, two measurements are almost uncorrelated for time-spacing of the order of 100 lattice sweeps. So we have decided to use the following scheme: In general, we ran a total of 150 000 iterations, discarding the first 50 000 iterations (to allow the system to reach equilibrium), and then taking measurements once every 100 lattice sweeps. Unless it is otherwise specified, the error bars have been obtained with several simulation runs, generally 8 or 16.

We have compared the two effective temperatures from the simulations with the corresponding temperature in the canonical ensemble. For two different temperatures, $\beta \approx 0.27$ which is far from the critical temperature $\beta_c = 0.4407$, and $\beta \approx 0.40$ closer to β_c, we have plotted the differences between the three methods, $\Delta\beta_{\mathrm{DLR,FF}} \equiv \beta_{\mathrm{DLR}} - \beta_{\mathrm{FF}}$, $\Delta\beta_{\mathrm{Cr,FF}} \equiv \beta_{\mathrm{Cr}} - \beta_{\mathrm{FF}}$, and $\Delta\beta_{\mathrm{Cr,DLR}} \equiv \beta_{\mathrm{Cr}} - \beta_{\mathrm{DLR}}$, as functions of $1/N$ for $n = 1$. We observe that, for both values of the temperatures, the three methods converge towards the same limit when the volume N increases (see figure 3). This confirms experimentally

the theoretical predictions for the microcanonical simulations, at large volume. Moreover, our results are compatible with a power law behaviour for the three differences, $\Delta\beta$: for $\beta \approx 0.27$ and $\beta \approx 0.40$, we have found $\Delta\beta = c \cdot N^{-\varpi(E,n)}$, with an exponent *a priori* depending on the ratio n, but which does not seem to vary with the energy (see figure 3). Actually, a least-squares fit of all data for $\Delta\beta_{\mathrm{DLR,FF}}$ gives $\varpi = 1.89 \pm 0.15$ for $\beta \approx 0.27$. At low temperature, the proportionality factor c is smaller for $\Delta\beta_{\mathrm{DLR,FF}}$ which means that the temperature computed from the (DLR) relation (3.3) is slightly better than Creutz's temperature, compared to the temperature of the canonical ensemble. If we do not know the exact solution for the system, we can define a 'thermalization' criterion for the simulations: $\Delta\beta_{\mathrm{Cr,DLR}}$ has to be as small as possible and has to decrease as L increases since at the thermodynamic limit $\beta_{\mathrm{DLR}} = \beta_{\mathrm{Cr}}$.

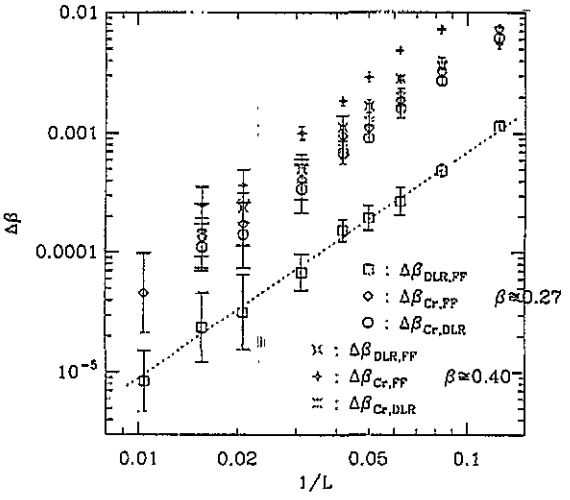

Figure 3. Comparison between the three different methods of computing the temperature. Three differences between the inverse temperatures are shown against $1/L$ for $n = 1$ near two temperatures $\beta \approx 0.27$ and $\beta \approx 0.40$. Error bars come from eight simulations runs. A slope of 1.89 is indicated in the figure.

We have also compared, for various ratios n, the temperature given by the simulations, either by DLR's or Creutz's methods, with the exact temperature computed from the exact canonical solution. In figure 4 we show, for a fixed volume of spins $N = 48 \times 48$, the relation of these two temperatures to the energy U of the Ising subsystem $\mathcal{I}$. We find a decrease in this difference $\Delta\beta_{\mathrm{DLR,FF}}$ with n at any temperature. This is in agreement with the result that when n tends towards infinity, the Ising subsystem $\mathcal{I}$ is described by a canonical Boltzmann distribution in which (DLR) relations are proven. We have also remarked that, first, $\Delta\beta_{\mathrm{DLR,FF}}$ is positive and grows when T tends towards T_c by the above values, and second, $\Delta\beta_{\mathrm{DLR,FF}}$ is negative and diminishes when T tends towards T_c by below values. Therefore there is a sharp variation in $\Delta\beta$ around T_c with a change of sign, but we have no explanation for this.

We have compared the microcanonical energy fluctuations for different values of n with the heat capacity of the exact canonical solution. The microcanonical energy fluctuations defined in the equation (3.4) $\tilde{C}_{48,n}$ for a 48×48 spin lattice are shown, for different values of n, together with the exact heat capacity for the corresponding two-dimensional Ising system in figure 5. Two important results are worth noticing. First, the difference between the simulations, and the exact solution, at a given temperature is smaller far from T_c, than it

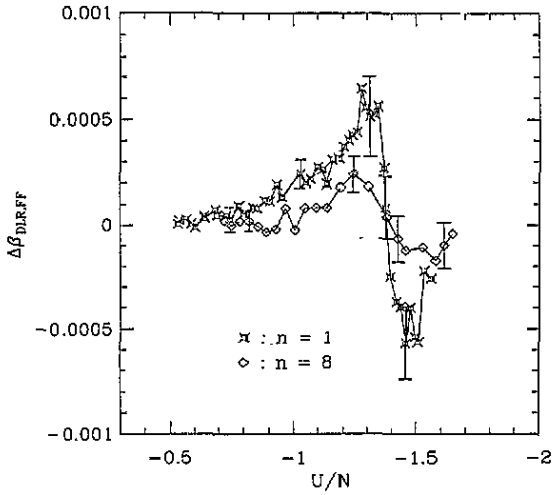

Figure 4. The difference between the inverse temperatures given by the exact solution and DLR's method against energy per site U, for a 48×48 lattice for $n = 1$ and $n = 8$. Error bars come from 16 simulation runs.

is near to T_c. Next, as the ratio n increases, the microcanonical energy fluctuations become closer to the canonical heat capacity at finite size. This is in agreement with the theoretical convergence of the spin system towards the canonical distribution, when n increases. At very large n the fluctuation–dissipation relation for energy should then be recovered.

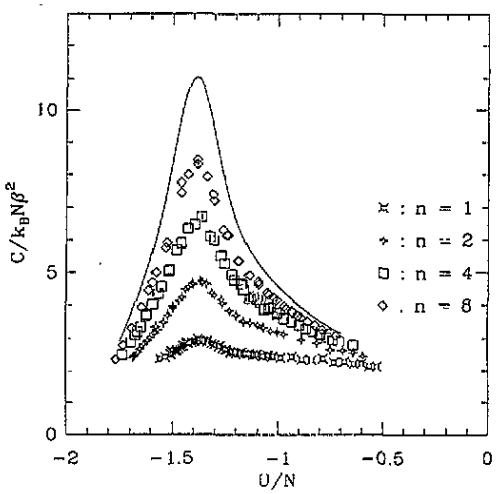

Figure 5. Microcanonical energy fluctuations per site divided by the square of the temperature $C/N\beta^2$, against the internal energy U/N, for a 48×48 lattice for different values of n. The full curve line represents the exact solution for the canonical heat capacity. Typical error bars are shown around $U/N = -1.4$ and $U/N = -1.0$; far from $U(T_c)$, error bars are smaller than the symbols.

Let us now analyse the microcanonical energy fluctuations $\tilde{C}$ at the critical temperature, compared to the size L of the lattice. Following the theory of finite-size scaling developed by Fisher (see [17] for a review), and the work of Ferdinand and Fisher [9], it is known that

$C(T_c)$ behaves as $A_0 \log(L)$ with $A_0 = (2/\pi)(\log((1+\sqrt{2}))^2 = 0.4945$. We experimentally observe a logarithmic variation of $\tilde{C}$ in function of the size L, with a proportionality factor strongly dependent on n (see figure 6). We have extracted this proportionality factor $A(n)$ defined by

$$C_{N,n}(T_c) = A(n)\log(L) + O(1) \tag{4.5}$$

where $N = L^2$ for a two-dimensional lattice. The proportionality constant $A(n)$ is found to increase with the number of demons, remaining between the null value and the canonical value A_0. This means that $(\Delta\mathcal{H}_\mathcal{I})^2$ has the same behaviour as the canonical heat capacity, up to a multiplicative constant $A(n)$ which tends, with increasing n, towards the canonical value. So the fluctuation–dissipation relation becomes valid for large n, in the microcanonical ensemble. We show the results in table 1.

Table 1. Proportionality factor A_n for various number of demons per spin n.

n	1	2	4	8	16	A_0
$A(n)$	0.0330	0.1063	0.2650	0.3305	0.3730	0.4945

We have found that the magnetization fluctuations in the simulations are compatible with fluctuations in the canonical ensemble. The susceptibility is then defined as $\chi = \partial M/\partial B = N\beta(\Delta M)^2$. The results are found to be in agreement with the classical results of [18], and do not seem to depend on the number of demons per spin, n. We have also analysed $|M|$ (the average on all the measurements of the absolute value of the magnetization of the Ising subsystem) as a function of $|T - T_c|$ for a given size L of the lattice (see figure 7). We have found the same results as Landau [18]. We have computed the scaling function X, where $|M|L^{\beta/\nu} = X(L^{1/\nu}|T - T_c|)$. For $T < T_c$ and large $x = L^{1/\nu}|T - T_c|$, it is known that $X(x) \approx Bx^\beta$. We have estimated the scaling exponent β of the X function with the hypothesis that, first we know T_c (the critical temperature of an infinite volume two-dimensional Ising system) and $\nu = 1$, and second, there is no dependence in n (that which is qualitatively checked). A least-squares fit of $\log(|M|L^{\beta/\nu})$ of all the data in the range $T \leqslant 0.98T_c$ yields $\beta = 0.106 \pm 0.012$ close to the theoretical value of $1/8$. Above T_c, a similar least-squares fit of all the data in the range $T \geqslant 1.02T_c$ yields the exponent $\tilde{\beta} = -0.866 \pm .009$ for the scaling function $X(x) \approx \tilde{B}x^{\tilde{\beta}}$, in good agreement with the result of $-7/8$.

We have also made a similar study for the susceptibility, computed with the fluctuations of the magnetization, and we find an ordinary scaling for χ:

$$\chi T \propto |1 - T_c/T|^{-\gamma} \qquad \text{for } T > T_c \tag{4.6}$$

and we find $\gamma = 1.744 \pm .016$ (with a least-squares fit of all data in the range $T > 1.1T_c$) in very good agreement with the theoretical value of $7/4$ (see figure 8).

5. Conclusion

The results presented here allow us to investigate a generalized 'microcanonical' algorithm, and to compare the results with the canonical results for a two-dimensional Ising lattice. We have shown experimentally that the two parts of the system, demons and lattice, are at equilibrium at the same temperature. We consider that these simulations constitute an experimental verification of ergodicity, but it remains to give a rigorous theoretical proof

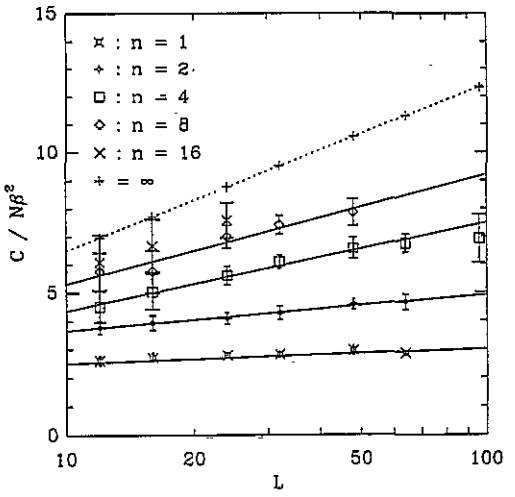

Figure 6. Finite-size scaling plot for the heat capacity—up to a multiplicative constant $1/N\beta^2$—at temperature T_c against the linear size L of the lattice, for several values of n. Plus signs represent the exact solution of Ferdinand and Fisher.

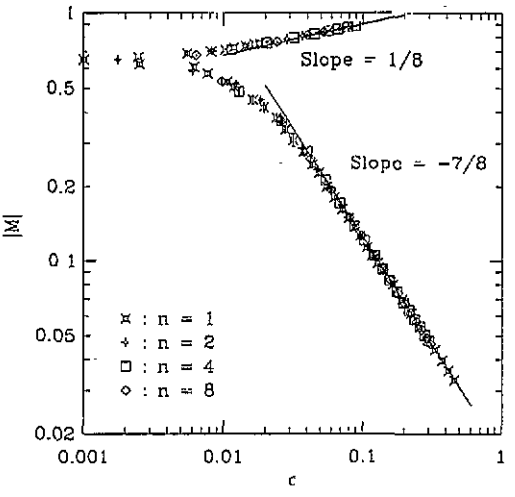

Figure 7. Finite-size scaling plot for the absolute value of magnetization against the reduced temperature ϵ, for a 48×48 lattice for different values of n. The upper data ($M \geqslant 0.55$) correspond to the temperatures below T_c ($\epsilon = 1 - T/T_c$), and the lower data correspond to the temperatures above T_c ($\epsilon = 1 - T_c/T$).

of the ergodicity for the microcanonical algorithm. We have shown how the fluctuations of the energy approach the canonical fluctuations when the set of demons begins to act as

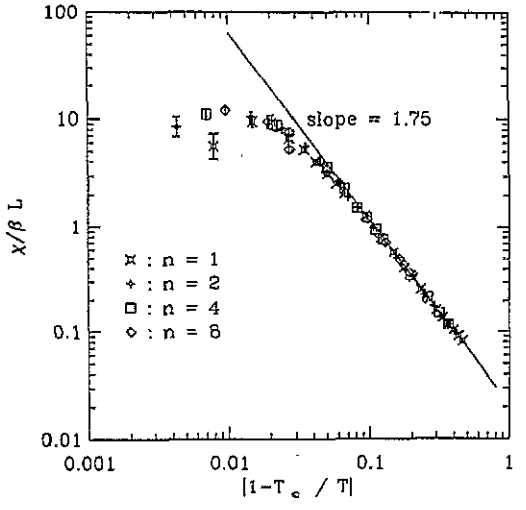

Figure 8. Finite-size scaling plot for the susceptibility against $1 - T_c/T$, for a 48×48 lattice for different values of n.

a thermostat. A new method to measure the temperature of the system has allowed us to define a 'thermalization criterion', measuring how close the microcanonical system is to the canonical ensemble. We believe further that this algorithm can be fruitfully applied to disordered systems such as spin glasses or to the random field Ising model where it can be extremely useful to average in a single 'valley'. Finally, we find experimentally that the dynamical exponent for the autocorrelation time is the same as that for the Metropolis Monte Carlo dynamics.

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Appendix A. Energy distribution of the Ising subsystem for large n

We show here that for N fixed, and n tending towards infinity, the Ising subsystem $\mathcal{I}$ adopts a canonical Boltzmann distribution for the energy.

The microcanonical distribution for the energy E is

$$\mathrm{d}P(\mathcal{I}, \mathcal{D}) = \delta(\mathcal{H}_\mathcal{I} + \mathcal{H}_\mathcal{D} - \mathcal{E})\,\mathrm{d}\mathcal{I}\,\mathrm{d}\mathcal{D}$$

which restricted to $\mathcal{I}$ (i.e. after integration over $\mathcal{D}$) becomes

$$\mathrm{d}P(\mathcal{I}) \propto W[E - \mathcal{H}_\mathcal{I}]\,\mathrm{d}\mathcal{I}$$

$$\int \mathrm{d}P(\mathcal{I}) = 1$$

where

$$W[E_{\mathcal{D}}] = \int \mathrm{d}P\,(\mathcal{D})\delta(E_{\mathcal{D}} - \mathcal{H}_{\mathcal{D}}).$$

Now when n is large, the volume $W[E_{\mathcal{D}}]$ of the fixed energy set of demons increases as

$$W[E_{\mathcal{D}}] = \sum_{l=\max(0,(E_{\mathcal{D}}-nN)/2)}^{\min(nN,E_{\mathcal{D}}/2)} \binom{nN}{l}\binom{nN}{E_{\mathcal{D}}-l} \propto \exp\left(ns\left(\frac{E_{\mathcal{D}}}{n}\right)\right)$$

where n goes to infinity at fixed ratio $E_{\mathcal{D}}/n = e$. The substitution of this result into the configuration probability of the Ising subsystem leads to

$$\mathrm{d}P(\mathcal{I}) \propto \mathrm{d}\mathcal{I}\exp\left(ns\left(e - \frac{\mathcal{H}_{\mathcal{I}}}{n}\right)\right) = \mathrm{d}\mathcal{I}\,\exp(-s'(e)\mathcal{H}_{\mathcal{I}})\exp(ns(e)).$$

This proves that the small Ising system has a canonical distribution with

$$\beta = \frac{\mathrm{d}s}{\mathrm{d}e}.$$

Appendix B. Equivalence between the microcanonical and Metropolis algorithms if the energy distribution of demons is Boltzmannian

We show here that if the distribution of demons is canonical then the microcanonical algorithm checks the detailed balance condition, and is equivalent to the Metropolis algorithm. Let $e^d_{\min} = 0$, and $e^d_{\max} = 3J$. The elementary moves $m_{i,k}$ can change the Ising energy by the following values: $\Delta\mathcal{H}_{\mathcal{I}} = 0, \pm J, \pm 2J$. The probability that a move involving a change of energy of $\Delta\mathcal{H}_{\mathcal{I}}$ is accepted is given by

$$\mathrm{P}(\Delta\mathcal{H}_{\mathcal{I}}) = \begin{cases} \mathrm{P}(e^d \geqslant \Delta\mathcal{H}_{\mathcal{I}}) & \text{if } \Delta\mathcal{H}_{\mathcal{I}} > 0 \\ 1 & \text{if } \Delta\mathcal{H}_{\mathcal{I}} = 0 \\ \mathrm{P}(e^d \leqslant 3J - \Delta\mathcal{H}_{\mathcal{I}}) & \text{if } \Delta\mathcal{H}_{\mathcal{I}} < 0. \end{cases}$$

The detailed balance condition regarding the canonical equilibrium distribution is easily checked for this probability of transition. For example, if $\Delta\mathcal{H}_{\mathcal{I}} = +J$, we have

$$\frac{\mathrm{P}(m_{i,k})}{\mathrm{P}(m_{i,k}^{-1})} = \frac{\mathrm{P}(\Delta\mathcal{H}_{\mathcal{I}})}{\mathrm{P}(-\Delta\mathcal{H}_{\mathcal{I}})} = \frac{\mathrm{P}(e^d \geqslant \Delta\mathcal{H}_{\mathcal{I}})}{\mathrm{P}(e^d \leqslant 3J - \Delta\mathcal{H}_{\mathcal{I}})} = \frac{\mathrm{e}^{-\beta J} + \mathrm{e}^{-2\beta J} + \mathrm{e}^{-3\beta J}}{1 + \mathrm{e}^{-\beta J} + \mathrm{e}^{-2\beta J}} = \mathrm{e}^{-\beta\Delta\mathcal{H}_{\mathcal{I}}}.$$

This proves that the microcanonical algorithm is equivalent to the Metropolis algorithm. This result can be extended to any value of e^d_{max}.

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