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Energy, fluctuation and the 2d classical XY-model

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Abstract : General analytical expressions on the fluctuation of the demon and system energy and the relationship between them have been established for microcanonical Monte Carlo simulations of systems with continuous symmetry These have been computationally verified for the 2d classical XY-model We suggest an alternative equilibration check and demonstrate that the system energy distribution is a Boltzmannian.

Keywords : Monte Carlo simulations, 2d XY-model, fluctuation

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Computer simulation has become very powerful and inevitable branch in theoretical physics of late. Use of different techniques for the study of model systems has increased its domain in its procedural prescriptions in simulations. One such prescription in this branch is the microcanonical Monte Carlo algorithm [1]. This technique interpolates between the Metropolis *et al* algorithm [2] and microcanonical formulation. Here, each one of the accessible microstates of the ensemble consisting of the spin system of interest alongwith the extra degree of freedom (the demon) is equally probable. The microcanonical MC algorithm thus simulates the sum :

$$Z = \sum \sum \delta\left[E_s(k) + E_d - E\right] \tag{1}$$

to generate a sequence of spin configurations k *via* the Markovian process where E is conserved. The system passes through a sequence of configurations with energy $E_s(k)$ having demon energy E_d in the phase space in a hopefully ergodic manner with the help of the demon. Although the composite system consisting of the demon and the system has microstates with constant total energy, individually the constituent parts suffer from fluctuation with respect to their energy.

E_d, in equilibrium, has the following distribution :

$$P(E_d) \sim \exp\left(E_d / k_B T\right) \tag{2}$$

Here T is the temperature of the spin system. k_B is set to be equal to unity. This distribution of E_d, when continuous, leads to the following analytical result :

$$\langle E_d^n \rangle / T^n = n! \tag{3}$$

where n is an integer.

The above equation and the constraint in eq. (1) lead to

$$\delta E_d^n = \sum_{i=2}^{n} (-1)^i n!/(n-i)!\, i!\, E^{(n-i)} \delta E_d^i \tag{4}$$

where i is an integer.

To verify eqs. 3 and 4 computationally, we consider a classical 2d XY-model with 225 and 900 spins witnessing the generalized potential [4],

$$H = 2J \sum_{\langle i j \rangle} \left[1 - \cos^{2p^2}\left((\theta_i - \theta_j)/2\right)\right] \tag{5}$$

where, all notations used have their usual meaning [3]. This Hamiltonian reduces to the usual classical 2d XY-system for $p^2 = 1$, undergoing the Kosterlitz-Thouless transition and with $p^2 = 50$ the system undergoes first order transition A single demon as the temperature controller and a square periodic bound lattice are the specifications for the system under study using the microcanonical Monte Carlo simulation technique. The simulation proceeds as has been described in one of our earlier papers [3]. The system is allowed to equilibrate for 1×10^5 MCSS and the averaging of the physical quantities has been done for 1×10^5 MCSS for $p^2 = 1$ and 50.

Figure 1 depicts the comparison of the equilibration of $\langle M^2 \rangle$ with that of $\langle E_d^n \rangle$ for $n = 2$, 3 and 4 (for $p^2 = 1$, $E = 519.3$ (E corresponds to a value close to the KT transition temperature) (1.a) and for $p^2 = 50$, $E = 1620.0$ (a value in the coexistence region of a first order transition) (1.b)) with 4×10^5 MCSS. The rate of equilibration of $\langle M^2 \rangle$ was found to get reduced when the change in $\langle M^2 \rangle$ between the initial stage and the final stage was large. For $p^2 = 50$, the change in $\langle M^2 \rangle$ is approximately the same for $E = 2160$ and 3060 and in this case the rate of equilibration of $\langle M^2 \rangle$ is fast when $\langle E_d \rangle = 2$ ($E = 3060$), the height of the potential well. This is attributed to the reduced width of the potential well for $p^2 = 50$. The system was found to be trapped quite often in metastable states for $p^2 = 50$, when the simulation was started with higher system energy. The metastable state consists of large regions of aligned spins. This situation can be circumvated by initially aligning a portion of the lattice and then starting the simulation. This essentially reduces the volume of the boundary between the regions of aligned spins. In this situation, $\langle E_d^n \rangle / T^n$ serves as an alternative check of equilibration.

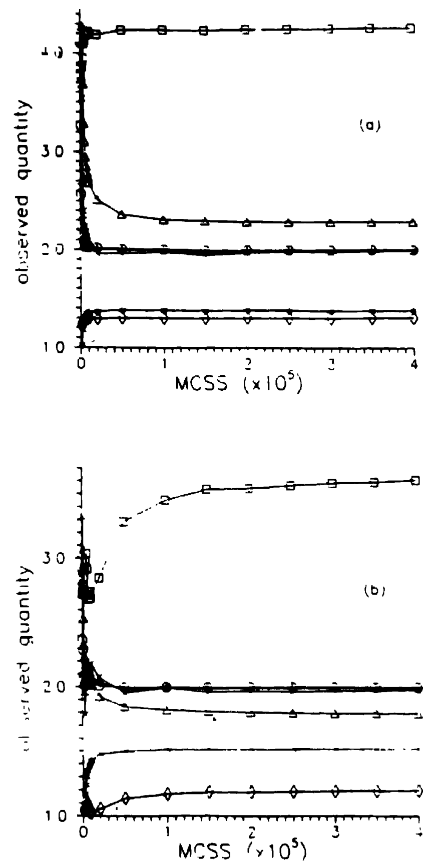

Figure 1. $2 \times \langle E_d^n \rangle / n! T^n$, for $n = 2$ (○), 3 (+) and 4 (×) and $10 \times N^{-2} < M^2 >$ (□), V (Δ), $3/2 \times < E_d >$ (∗) and $2 \times < M >$ (◊) as functions of MCSS for 30×30 spin system. Each data point represents the average over the configurations up to a given MCSS. The continuous line is a guide to the eye. The initial configuration were with all spins parallel to each other (a) $p^2 = 1$, $E = 519.3$, $T = 0.918$ and V is scaled to $V/2$, (b) $p^2 = 50$, $E = 1620.0$, $T = 1.01$ and V is scaled to $V/20$.

Table 1 depicts $\langle E_d^n \rangle / T^n$ for $n = 2$, 3 and 4 and for the spin system with 225 and 900 spins. This estimates δE_s^n using eq. (4). Here, we observe that, $\langle E_d^n \rangle / T^n$ is close to n ! and deviation from n ! value increases as n increases for a given system size and is more for smaller system size. $\delta E_s^2 / T^2$ is observed to be a straight line parallel to X-axis at $Y = 1$ which is contrary to the conventional nature (a peak at a usual transition temperature). We also find that $\delta E_d^2 / T^2 = 1$. From the simulation result, we infer that the mean square fluctuation of the demon and the system energy are the same and it is found that the system energy distribution is reflected through the demon energy distribution. The standard deviation of various quantities are given within bracket in the table.

In conclusion, we obtained a simple relationship between the fluctuations of the system- and the demon-energy for systems with continuous symmetry analytically in a microcanonical framework and demonstrated it for the case of the classical 2d XY-model.

Table 1. Values of E, T and $\langle E_d^n \rangle / T^n$ with $p^2 = 1$ and 50.

System size	p^2	1			50		
	E	60.7	129.8	310.3	67.5	405	742.5
	T	0.4986	0.9222	1.7552	0.5280	1.0286	1.6170
		(± 0.0041)	(± 0.0098)	(± 0.0241)	(± 0.0065)	(± 0.0123)	(± 0.0216)
15 × 15	$\langle E_d^2 \rangle / T^2$	1.979	1.988	1.984	1.989	2.002	1.978
		(+ 0.074, − 0.071)	(+ 0.097, − 0.094)	(+ 0.122, − 0.116)	(+ 0.103, − 0.098)	(+ 0.104, − 0.100)	(+ 0.111, − 0.106)
	$\langle E_d^3 \rangle / T^3$	5.821	5.901	5.834	5.892	6.032	5.802
		(+ 0.411, − 0.394)	(+ 0.535, − 0.506)	(+ 0.646, − 0.601)	(+ 0.529, − 0.496)	(+ 0.558, 0.524)	(+ 0.569, − 0.531)
	$\langle E_d^4 \rangle / T^4$	22.66	23.22	22.57	23.13	24.24	22.46
		(+ 2.88, − 2.71)	(+ 3.79, − 3.51)	(+ 4.16, − 3.78)	(+ 3.40, − 3.12)	(+ 3.67, 3.38)	(+ 3.58, − 3.26)
	E	243.0	519.3	1241.1	270	1620	2970
	T	0.4986	0.9165	1.7815	0.5275	1.0175	1.6442
		(± 0.0056)	(± 0.0120)	(± 0.0267)	(± 0.0029)	(± 0.0164)	(± 0.0241)
30 × 30	$\langle E_d^2 \rangle / T^2$	2.003	2.003	1.994	2.001	2.005	1.987
		(+ 0.098, − 0.094)	(+ 0.106, − 0.101)	(+ 0.121, − 0.115)	(+ 0.055, − 0.054)	(+ 0.141, − 0.133)	(+ 0.126, − 0.120)
	$\langle E_d^3 \rangle / T^3$	6.011	6.017	5.939	5.996	6.055	5.875
		(+ 0.538, − 0.507)	(+ 0.575, − 0.538)	(+ 0.635, − 0.588)	(+ 0.348, − 0.338)	(+ 0.727, − 0.669)	(+ 0.620, − 0.575)
	$\langle E_d^4 \rangle / T^4$	24.15	24.08	23.43	23.82	24.52	22.88
		(+ 3.88, − 3.58)	(+ 4.06, − 3.70)	(+ 4.20, − 3.78)	(+ 2.64, − 2.54)	(+ 4.70, − 4.21)	(+ 3.81, − 3.45)

Although, this equation is independent of the order of transition and the number of extra degrees of freedom, we undertook the present study with a single demon. We prescribe $E_d^n / T^n = n!$ as an alternative equilibration check in a microcanonical framework for continuous systems in specific circumstances. We also observe that the system energy distribution is a Boltzmannian when the system is controlled by a single demon.

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