Importance of starting configurations in Q2R: temperature measurement

1989 J. Phys. A: Math. Gen. 22 4487

(http://iopscience.iop.org/0305-4470/22/20/024)

J. Phys. A: Math. Gen. 22 (1989) 4487–4491. Printed in the UK

COMMENT

Importance of starting configurations in Q2R: temperature measurement

C Moukarzel
Centro Atómico Bariloche, 8400 Bariloche, Republic of Argentina

Received 18 April 1989

Abstract. The incorrect local energy distribution given by Q2R at low temperatures is shown to be due to the non-microcanonical character of the starting states. Correct measurements are obtained with microcanonically distributed starting configurations. The probable behaviour of the dynamics for large lattices is also discussed.

One of the open questions concerning Q2R is its failure to give correct local energy distribitions at low energies [1]. The local energy e is defined as minus the product of the spin and the internal field at a given site. Its distribution $P(e)$ for the zero-field Ising model in the canonical ensemble satisfies $P(-e)/P(e)=\exp(2\beta e)$. One can see that this result also holds in the microcanonical (μC) ensemble at fixed energy E, identifying β as the coupling at which the average energy in the canonical ensemble is E.

To show this let us define

$$\beta_e = (1/2e)\ln(P(-e)/P(e)). \tag{1}$$

In the microcanonical ensemble one has $P(e)=G(E,e)/G(E)$ with $G(E)$ being the number of states with energy E and $G(E,e)$ the number of those with local energy e at a fixed site. Using the identities $G(E,-e)=G(E+2e,e)$; $G(E)=\exp(S)$, expanding in powers of $2e$ and renaming $\mathrm{d}S/\mathrm{d}E=\beta$, we finally obtain

$$\beta_e = \beta + \left(e\frac{\mathrm{d}\beta}{\mathrm{d}E}+\frac{\mathrm{d}\ln(P(e))}{\mathrm{d}E}\right)+\mathrm{O}(N^{-2}) \tag{2}$$

so in the microcanonical ensemble, (1) makes $\mathrm{O}(1/N)$ corrections to β.

In the 2D Ising model the local energy can take the values 4, 2, 0, −2, −4, so one has two independent relations allowing the measurement of β. They are

$$T1=[\tfrac{1}{8}\ln(P(-4)/P(4))]^{-1} \tag{3}$$

$$T2=[\tfrac{1}{4}\ln(P(-2)/P(2))]^{-1}. \tag{4}$$

$T1$ and $T2$ were measured in Q2R and the resulting deviations $\Delta T1=(T1-T)$ and $\Delta T2=(T2-T)$ are shown in figure 1 for $(64)^2$ and $(128)^2$ lattices. The correct temperature T was extracted from the Onsager relation $E(\beta)$. The data were obtained by making 1000 Q2R steps from each of 20 different starting configurations of energy $E(\beta)$, constructed by flipping spins at random positions from the ordered state until the desired energy was reached (type-I starting states).

0305-4470/89/204487+05$02.50

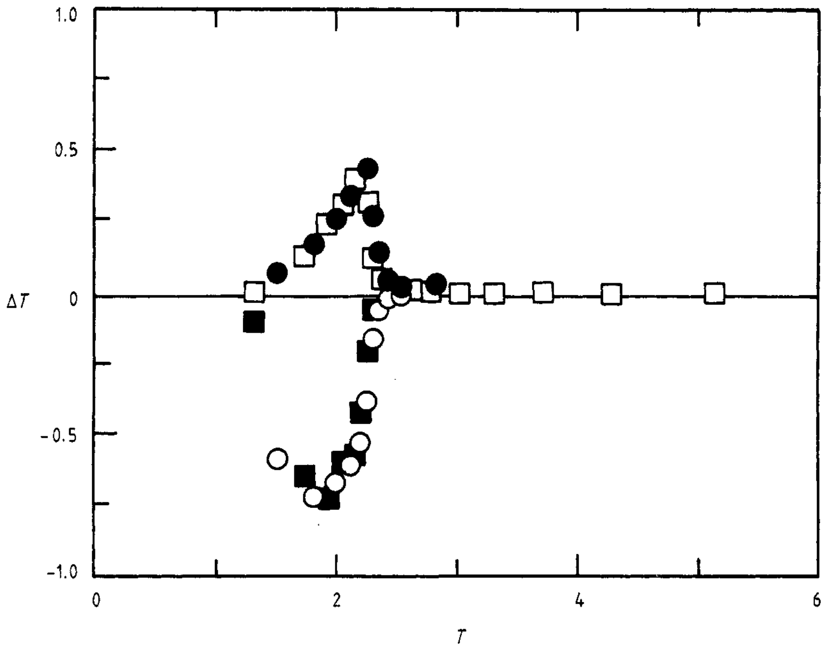

Figure 1. Deviations $\Delta T1 = (T1 - T)$ and $\Delta T2 = (T2 - T)$ measured with 1000 Q2R steps from 20 type-I starting configurations for $L = 64$ ($\Delta T1$: □, $\Delta T2$: ■) and $L = 128$ ($\Delta T1$: ●, $\Delta T2$: ○).

It is apparent from the data that the observed deviations at low temperature are not $O(1/N)$ corrections.

The dependence of the results on the observation times was tested by repeating the calculations with 10^2, 10^3, 10^4, and 10^5 Q2R steps for $L = 32$, 64, and 128. A slow relaxation was observed at $T = 2.177$, 2.234, and 2.276, in accordance with previous findings of Stauffer [2].

The relaxation shows a slowing down as T decreases. Only at $T = 2.276$ were correct values for $T1$ and $T2$ reached after 10^5 iterations. No relaxation was detected for $T < 2$. A time dependence over a greater period of time than the one tested is not possible for this lattice size at low temperatures because global periods are not long enough. Then we conclude that the deviations at low temperature are not an effect of short observation times, at least for this lattice size.

Let us see what the properties are of the starting configurations we have used in the simulation. To test this, $T1$ and $T2$ were measured on initial states only, i.e. with no Q2R updating. The configurations, 100 at each energy, were obtained by the method already described (method I) and the results are shown in figure 2. It is now evident that this method does not yield microcanonically distributed states. The serious problem is that at low temperatures Q2R does not 'erase' the non-microcanonical characteristics of the starting states.

One of the hypothesis one makes when measuring with Q2R is that the time-averaged magnitudes are independent of any atypical characteristics of the starting configurations. This seems to hold well for magnetisation [3, 4] and susceptibility [5] measurements but it has been already observed that the choice of starting states is not irrelevant in the evaluation of the staggered magnetisation [6]. The same happens in this case.

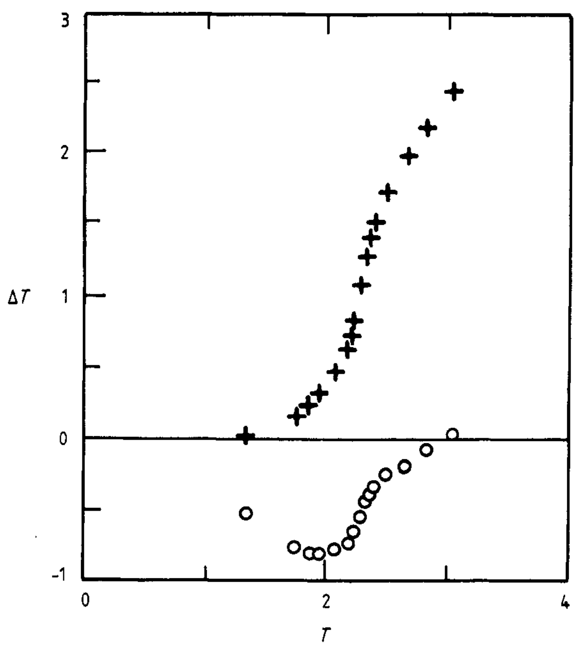

Figure 2. Deviations $\Delta T1$ and $\Delta T2$ measured on 100 type-I starting configurations for $L=64$ ($\Delta T1$: +, $\Delta T2$: ○).

There are some characteristics of the starting states obtained by method I which seriously affect the measurement of $T1$ and $T2$ and are not overridden by the dynamics (owing, of course, to its strongly non-ergodic character) at low temperatures.

A method for obtaining microcanonically distributed states with energy E is the following. First invert $E(\beta)$ to extract β. Then thermalise the system in the canonical ensemble at inverse temperature β (by Monte Carlo means). The energy will fluctuate around its average value E. Select a state with energy E. Repeating this procedure, one gets a set of states with energy E and microcanonical distribution.

Taking such a set as the starting configurations for the simulation with Q2R, one obtains coincidence between T, $T1$, and $T2$ within statistical error. This is shown in figure 3 for $L=64$. Analogous results were found for $L=128$. The data were obtained by averaging over 1000 Q2R steps from 40 microcanonical starting configurations.

This result is in accordance with previous claims [5] that Q2R should correctly reproduce any microcanonical ensemble result if certain conditions, one of them being the microcanonical distribution of starting states, are met in the simulation.

In the case when the conditions on the starting configurations are not fulfilled, for example when type-I starting states are used, it is not yet clear whether the deviations T will remain non-zero for all lattice sizes or if the non-ergodic zone will be progressively confined to lower temperatures as the lattice size is increased. The average 'mobility' V, defined as the fraction of sites with zero internal field, gives us an estimation of the fraction of spins that change their state at each Q2R step. We can see in figure 4 that this magnitude drastically drops at low temperatures so there many more Q2R steps would be needed in order to obtain a configuration that substantially differs from the starting one. However, at low temperatures global periods are short, so the system never gets far from the starting point, and the measurements depend strongly on the

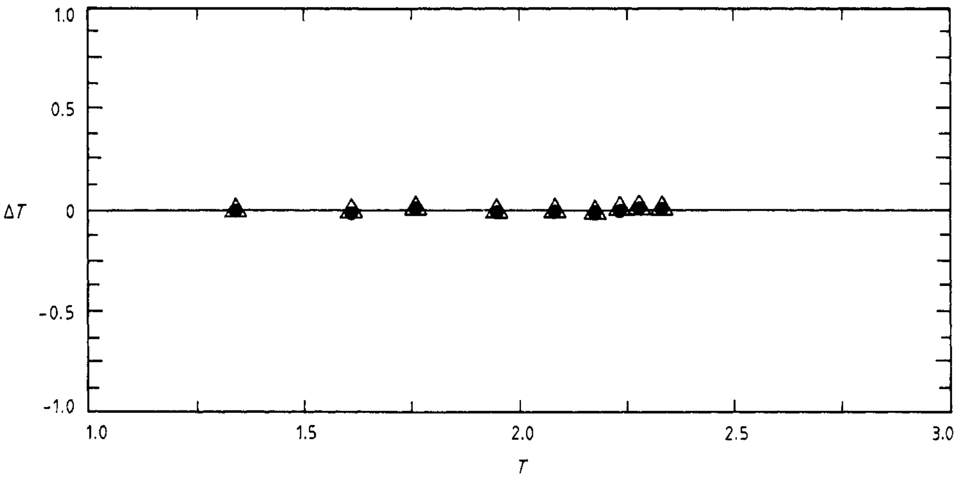

Figure 3. Deviations $\Delta T1$ and $\Delta T2$ measured with 1000 Q2R steps from 40 microcanonically distributed starting states for $L = 64$ ($\Delta T1$: ●, $\Delta T2$: △).

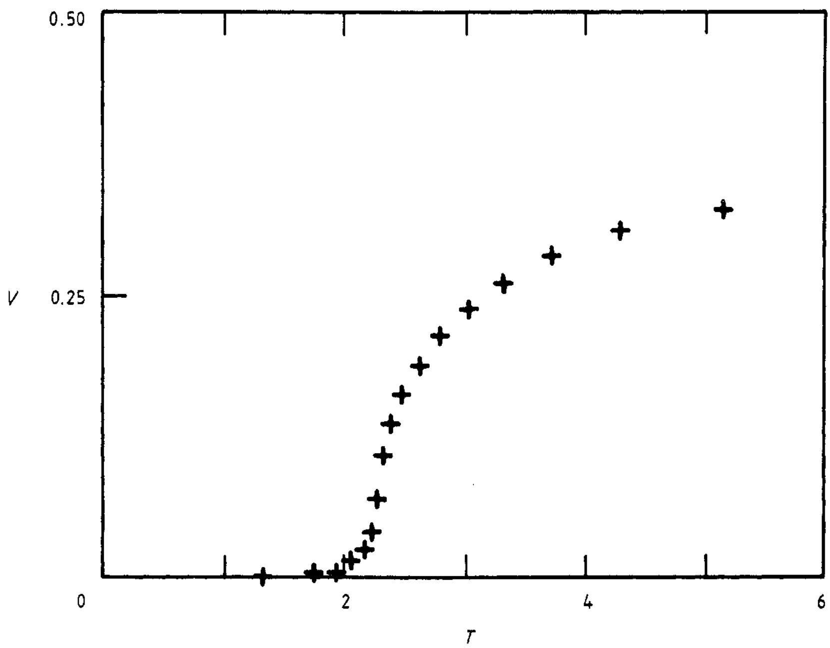

Figure 4. Mobility plotted as a function of temperature measured with 1000 Q2R steps from ten type-I starting states for $L = 64$.

properties of the starting configurations. Increasing the lattice size at fixed temperature makes the cycles longer, so in principle the dynamics might be able to exhibit improved ergodicity in the limit of large lattice and large observation time, but this is still an open question. Let us, however, remark that if the cluster picture at low temperature [7] is valid then it is not the global cycle length but the average cluster period which is relevant to determining the time dependence of the measured magnitudes, and this magnitude has only a mild growth with L, if any, so if ergodicity is improved in some large-L limit, it will only be so for much larger lattices than the ones studied in this work.

As a final observation, and in view of the importance of the starting states distribution at low temperatures, let us note that it would be of interest to analyse how the picture of the ergodicity transition [7] is modified if only microcanonical starting configurations are used.

Acknowledgment

The author is supported by a fellowship granted by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET).

References

[1] Lang W M and Stauffer D 1987 *J. Phys. A: Math. Gen.* **20** 5413
[2] Stauffer S 1988 private communication
[3] Herrmann H J 1986 *J. Stat. Phys.* **45** 145
[4] Zabolitzky J and Herrmann H 1988 *J. Comput. Phys.* **76** 426
[5] Moukarzel C and Parga N 1989 *J. Phys. A: Math. Gen.* **22** 943
[6] Costa U and de Cruz H 1987 *Preprint* Universidad Federale de Alagoas
[7] Herrmann H J, Carmesin H O and Stauffer D 1987 *J. Phys. A: Math. Gen.* **20** 4939