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On the evaluation of magnetisation fluctuations with Q2R cellular automata

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Abstract. We discuss the evaluation of fluctuations with the Q2R cellular automata. Explicit calculations are performed for the two-dimensional case. We argue that when Q2R results are compared properly with Monte Carlo simulations there are no inconsistencies at low temperatures as claimed recently.

1. Introduction

A cellular automaton (Wolfram 1984) consists of a finite set of N discrete variables σ_i $(i=1,\ldots,N)$, the temporal evolution of which is dictated by a rule of the general form

$$\sigma_i^{t+1}=\Phi_i(\{\sigma^t\}). \tag{1}$$

In Q2R automata (Pomeau 1984) the σ are Ising variables defined on a square $L\times L$ lattice with nearest-neighbour interactions. The dynamics is such that spins are flipped only when they have as many neighbours up as down. Dividing the system into two interpenetrating lattices in such a way that each site of one sublattice has its neighbours on the other sublattice, the updating may be done for all the variables on a sublattice simultaneously while conserving the energy. Then, updating the sublattices one at a time, one supposedly has a microcanonical (μC) simulation of the Ising model. The algorithm can be readily generalised to higher dimensionalities or to non-nearest-neighbour interactions. In this last case the number of sublattices in which the system is split must be greater than two in order to ensure that no site interacts with another on its own sublattice. The possibility of simultaneous update and the deterministic character of this algorithm (no random numbers are needed) allow high-speed simulations, with 4.3×10^9 spin-flip attempts per second on a Cray (Herrmann 1986, Zabolitzky and Herrmann 1987). While the spontaneous magnetisation of the Ising model is well reproduced by this algorithm, it is not yet certain (Herrmann *et al* 1987, Lang and Stauffer 1987) under which conditions Q2R automata can be regarded as equivalent to the Ising model.

Recently Lang and Stauffer (1987) found for the three-dimensional Q2R automata what they interpreted to be a deviation from the expected behaviour of the zero-field susceptibility χ measured through

$$\chi=N\beta\langle\Delta M^2\rangle \tag{2}$$

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with

$$\langle \Delta M^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2 \tag{3}$$

and

$$M = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tag{4}$$

and compared with Monte Carlo (MC) results.

In this work we stress the fact that in a μC ensemble the zero-field susceptibility χ is not given by (2) because magnetisation fluctuations are not independent of the ensemble (Lebowitz 1967) while χ is. Fluctuations in a μC ensemble differ from those given by MC simulations by a correction term which is relevant even in the thermodynamic limit. We calculate the correction using MC and show that Q2R gives, in the limit of large lattices, the expected result for magnetisation fluctuations in a μC ensemble. We work with two-dimensional lattices but we expect the same to be valid in three dimensions.

As a different but related topic, we compare several methods of measuring with Q2R automata and make some suggestions which could help to clarify the equivalence between the Ising model and Q2R automata.

2. General observations

2.1. *Fluctuations in a μC ensemble*

The first thing one has to notice is that while expectation values of extensive magnitudes are independent of the ensemble in the limit $N \to \infty$, this is no longer true for the average value of fluctuations, which do possess a dependence on the ensemble (Lebowitz 1967). The simplest example of this is given by energy fluctuations which of course vanish in a μC ensemble but are related to the specific heat in a canonical ensemble.

Let us denote by $\langle \ \rangle_\beta$ and $\langle \ \rangle_E$ the canonical and μC ensemble averages respectively. If there is no subscript, an arbitrary ensemble is understood.

The zero-field susceptibility

$$\chi = \lim_{h \to 0} \frac{\partial \langle M \rangle}{\partial h} \tag{5}$$

where h stands for the external magnetic field, is not given by (2) when the averages are taken in a μC ensemble because $N\langle \Delta M^2 \rangle_E$ has an O(1) correction with respect to the canonical ensemble.

Let us define

$$\theta(\beta) = N\beta \langle \Delta M^2 \rangle_E \tag{6}$$

where the μC average is taken at the value of the energy which satisfies

$$E(\beta) = \langle E \rangle_\beta . \tag{7}$$

Then the following relation holds (see appendix):

$$\theta(\beta) = \chi(\beta) - N\beta \frac{\langle \Delta E \Delta M \rangle_\beta^2}{\langle \Delta E^2 \rangle_\beta} + \mathrm{O}(1/N). \tag{8}$$

Let us note that the correction term remains finite in the thermodynamic limit. This implies that the conclusions of Lang and Stauffer (1987) are unfounded since they compare θ with χ disregarding this term.

We conclude that the average value of fluctuations obtained with the Q2R cellular automata should be compared with the same magnitude estimated with a μC ensemble. In practice what we shall do is to calculate $\theta(\beta)$ by means of MC simulations using (8) to evaluate the correction. Let us remark, however, that apart from that term there are also finite-size corrections $O(1/N)$; because of this the automata will become comparable to the estimated μC fluctuation only for large N.

2.2. *On how to measure with Q2R*

Because of the reversibility and deterministic character of this algorithm each spin configuration belongs to a cycle, i.e. the initial configuration is recovered after l updatings, where l is the length of the cycle (Herrmann 1986, Herrmann *et al* 1987). For this reason if one starts from a given phase-space point the only accessible configurations are those which belong to the same cycle as the initial point. This means that the Q2R automata generate phase-space points with a weight which is not truly μC. Of course this does not mean that Q2R cannot be used to calculate μC averages. It is clear that if one could complete all cycles with a fixed energy once, then all configurations with that energy would be reached with even weight. As one cannot do that in practice, it is necessary to decide how to measure. Since different choices can lead to different averages, we will analyse which ones are correct and easy to implement.

Let us suppose one decides to take as a phase-space sampling the set of configurations obtained by completing a given number, P, of cycles. The corresponding P starting configurations are chosen with μC weight at that energy and with a magnetisation of definite sign. This means that the probability for a given cycle to be selected is proportional to its length l; as a result, phase-space points are generated with a weight proportional to the length of the cycle containing that configuration. For this reason the μC average will not be obtained as a direct average over the whole set of configurations generated in that way; rather one has to take a weighted average with a factor $1/l$ to compensate for the fact pointed out above. This turns out to be equivalent to assigning to each starting configuration the average value calculated on its cycle and then averaging over initial configurations (or cycles) with equal weights (see equation (9)).

An alternative way to take averages with correct μC weights is to select P cycles and to consider a fixed number, K, of updatings in each of them. As before the probability for a cycle to be selected is proportional to l, but now the probability for a given configuration within that cycle to be reached is K/l. The factors cancel out and configurations appear with even weights.

Both methods reduce to

$$\langle F\rangle_{\mathrm{Q2R}}=\left(\frac{1}{P}\right)\sum_{s=1}^{P}\langle F\rangle_s \qquad (9)$$

where $\langle F\rangle_s$ is the average of F on the whole or a part of cycle s.

We have tested both methods and have found that they yield similar results for the magnetisation fluctuations as long as K is not too small.

Apart from what we have just pointed out, let us remark that it is not correct to take the single-cycle magnetisation fluctuation as representative of the μC average. The reason for this is that it would be an underestimation of the μC value because we will not be considering the intercycle fluctuations. This can be easily shown.

Let us denote the single-cycle value of $\langle\Delta M^2\rangle$ by δ_s and with its average over cycles by δ_1:

$$\delta_s = \langle\Delta M^2\rangle_s = \langle M^2\rangle_s - \langle M\rangle_s^2 \tag{10}$$

$$\delta_1 = \bar{\delta}_s = \frac{1}{P}\sum_{s=1}^{P} \delta_s \tag{11}$$

where $\langle\ \rangle_s$ means average over the configurations belonging to the cycle s and the overbar denotes the average over cycles.

On the other hand, the total fluctuations calculated over the whole set of the generated configurations are (using (9)):

$$\delta_2 = \langle M^2\rangle - \langle M\rangle^2 = \left(\frac{1}{P}\sum_s \langle M^2\rangle_s\right) - \left(\frac{1}{P}\sum_s \langle M\rangle_s\right)^2 \tag{12}$$

then

$$\delta_2 - \delta_1 = \overline{\langle M\rangle_s^2} - \overline{\langle M\rangle_s}^2 \tag{13}$$

which proves the statement above.

As a consequence of this fact, if the intercycle fluctuations are important, one will never get a correct estimate of their total value by averaging on one cycle only. As we shall see at the end of the next section, this is indeed the case at low temperatures.

3. Numerical results

Motivated by the observations of § 2, we measured $\theta(\beta)$ with Q2R using (6) and with MC using (8). Both programs were written using multispin coding (Jacobs and Rebbi 1981, Williams and Kalos 1984). For the MC program we used a version of multispin coding similar to that of Williams and Kalos (1984) where the whole updating process is done in parallel.

Monte Carlo results for magnetisation fluctuations were obtained updating the whole lattice 12 000 times at each temperature, discarding the first 2000 iterations to allow for thermalisation, and then measuring M and E after each tenth MC step.

The link between the canonical ensemble with fixed β and the μC ensemble with fixed E is made by taking the MC energy to be the mean value $\langle E\rangle_\beta$ obtained in the canonical ensemble at inverse temperature β. For Q2R simulations we used the exact relation (Huang 1963) to obtain β from E. We estimated $\langle M\rangle$ and $\langle M^2\rangle$ using (9) and averaging over 20 different cycles at each value of the energy. The initial configurations were obtained from the ordered state by flipping spins at random locations till the desired value of E was reached. On each cycle the system was updated 10 000 times and M was measured after every updating. The simulation was finished on those cycles where the starting configuration was reached again before 10 000 updatings.

In figure 1 we show our results for the magnetisation fluctuations. For comparison purposes we include our MC data for χ, the μC value θ calculated using (8), and Q2R results for different values of L. The Monte Carlo and the corresponding μC estimate are shown for our largest lattice, $L = 64$, only.

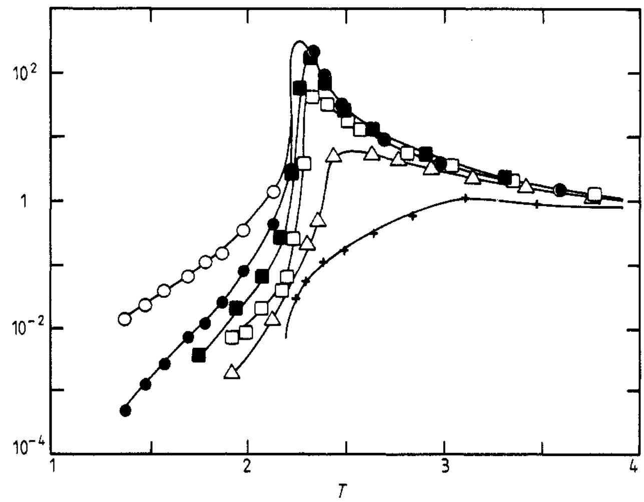

Figure 1. Magnetisation fluctuation data for canonical (○) and microcanonical (●) ensembles calculated by Monte Carlo for $L = 64$, and Q2R magnetisation fluctuations for $L = 6$ (+), $L = 10$ (△), $L = 20$ (□) and $L = 64$ (■).

Let us notice that even at the largest size we considered there is still a difference between the estimated μc and the Q2R results. This could be attributed to the $O(1/N)$ correction terms to the μc data coming from the change of ensemble (see equation (8)), not included in figure 1. Let us give, however, a word of caution; there is still the possibility that the dynamics of the automaton itself introduces other finite-size effects or, even worse, $O(1)$ differences with respect to an exact μc. Our data, however, do not rule out the consistency between Q2R magnetisation fluctuations and the two-dimensional Ising model.

As discussed in § 2.2, the intercycle fluctuations may give a relevant contribution to the susceptibility. This is shown to be true in figure 2, where we show the relative

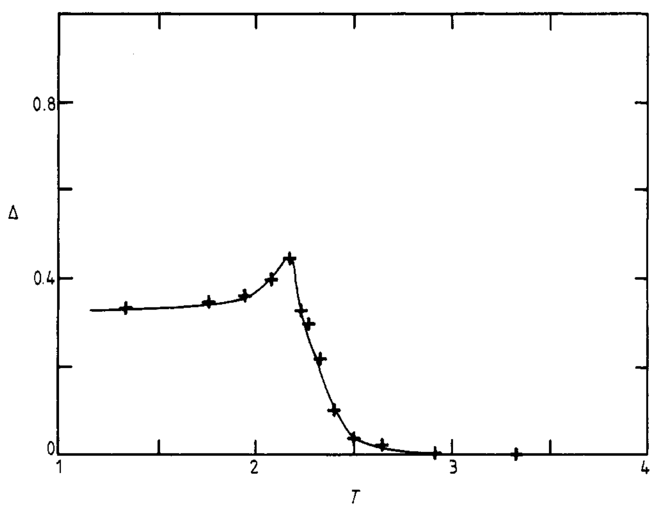

Figure 2. Relative intercycle fluctuations Δ plotted against temperature for Q2R with $L = 64$.

intercycle fluctuation Δ

$$\Delta = (\delta_2 - \delta_1)/\delta_2 \tag{14}$$

as a function of temperature. The data in figure 2 are for $L = 64$, but we found a similar behaviour on the other lattices. In general, the intercycle fluctuations are half the total fluctuations at low temperature but vanish approximately at the point where the total fluctuations coincide with MC results.

4. Conclusions

We have shown that the magnetisation fluctuations for the Ising model in a μC ensemble differ from the canonical value for $T < T_c$. For that reason, it is not correct to compare Q2R fluctuations with MC fluctuations directly; rather, these have to be corrected in order to estimate the μC averages. Once this correction is considered, Q2R still fails to give the μC values for the magnetisation fluctuations, but our data suggest that the remaining differences may be finite-size effects.

As has already been observed (Herrmann 1986, Herrmann *et al* 1987), in order to obtain a good estimate of a given quantity one has to take into account the contributions of many cycles. We have seen that for $\langle M \rangle$ (and so for $\langle \Delta M^2 \rangle$, see equation (13)) this is necessary only at low temperature where our data show that the intercycle fluctuations represent a substantial fraction of $\langle \Delta M^2 \rangle$. At higher temperature this contribution becomes negligible so a single cycle average is enough.

We have also tested the dependence of the observed fluctuations on the number, K, of the updatings that one does on each cycle and we found that near T_c the values for $K = 1000$ and $K = 10\,000$ differ (figure 3). This effect was not observed (with the same values for K) in our smaller lattices, for which the mean cycle lengths were not too big at that temperature. For this reason we expect that in order to obtain an approximation to the complete cycle average, K should not be taken too small compared with the cycle length. This would imply that the required observation times grow

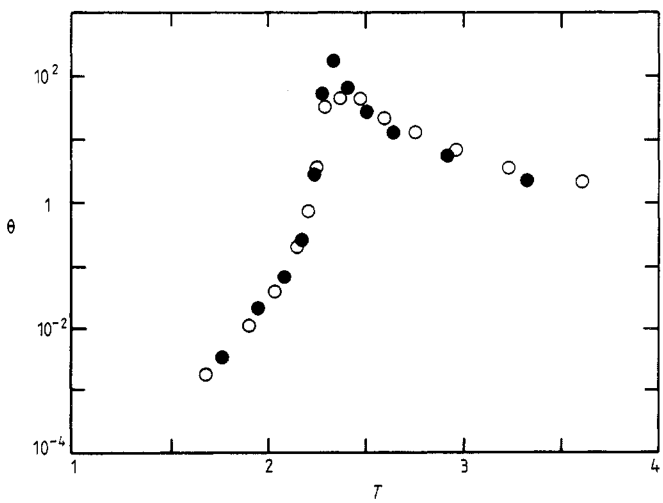

Figure 3. Dependence of the observed fluctuations on the number, K, of iterations per cycle for Q2R with $L = 64$. The data shown correspond to $K = 1000$ (○) and $K = 10\,000$ (●).

strongly with N near T_c and this fact, together with the necessity of averaging over several cycles, might make the efficiency of the algorithm uncertain.

Appendix

Here we sketch the derivation of (8). For a discussion in the case of more general ensembles, see Lebowitz (1967).

Let us denote the μC average of F by $\langle F\rangle_E$:

$$\langle F\rangle_E = \frac{1}{g(E)}\sum_r \delta(E_r - E)F_r \tag{A1a}$$

with

$$g(E) = \sum_r \delta(E_r - E) \tag{A1b}$$

where Σ_r stands for a sum over the whole phase space of the system.

Analogously, $\langle F\rangle_\beta$ is the canonical average

$$\langle F\rangle_\beta = \frac{1}{Z(\beta)}\sum_r \exp(-\beta E_r)F_r \tag{A2a}$$

with

$$Z_{(\beta)} = \sum_r \exp(-\beta E_r). \tag{A2b}$$

Then it is easily shown that

$$\langle F\rangle_\beta = \frac{1}{Z(\beta)}\int_0^\infty \mathrm{d}E\, \exp(-\beta E)g(E)\langle F\rangle_E. \tag{A3}$$

Expanding $\langle F\rangle_E$ in powers of $(E-\bar{E})$ (where $\bar{E} = \langle E\rangle_\beta$), we obtain

$$\langle F\rangle_\beta = \langle F\rangle_E - \tfrac{1}{2}\frac{\partial E}{\partial\beta}\frac{\partial^2\langle F\rangle_E}{\partial E^2} + \mathrm{O}(\langle F\rangle/N^2) \tag{A4}$$

where all functions of E are evaluated at $\bar{E}$.

One can readily see that the term

$$\frac{\partial E}{\partial\beta}\frac{\partial^2\langle F\rangle}{\partial E^2}$$

vanishes like $1/N$, so in the thermodynamic limit we obtain the same average in both ensembles.

Now, in the case of fluctuations

$$\langle \Delta F\Delta G\rangle = \langle (F-\langle F\rangle)(G-\langle G\rangle)\rangle = \langle FG\rangle - \langle F\rangle\langle G\rangle \tag{A5}$$

applying (A4) to the right-hand side of (A5), we have

$$\langle \Delta F\Delta G\rangle_\beta = \langle \Delta F\Delta G\rangle_E - \frac{\partial E}{\partial\beta}\frac{\partial\langle F\rangle_E}{\partial E}\frac{\partial\langle G\rangle_E}{\partial E} + (\langle\Delta F\Delta G\rangle/N). \tag{A6}$$

Here the correction term

$$\frac{\partial E}{\partial \beta} \frac{\partial \langle F \rangle}{\partial E} \frac{\partial \langle G \rangle}{\partial E}$$

is of the same order, $1/N$, as $\langle \Delta F \Delta G \rangle$ itself.

For the case of magnetisation fluctuations both F and G are M, so approximating $\langle M \rangle_E$ by $\langle M \rangle_\beta$ (to the same order), we obtain

$$\langle \Delta M^2 \rangle_\beta = \langle \Delta M^2 \rangle_E + \frac{\langle \Delta E \Delta M \rangle_\beta^2}{\langle \Delta E^2 \rangle_\beta} + \mathrm{O}(\langle \Delta M^2 \rangle / N) \qquad \text{(A7)}$$

from which (8) stems.

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