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Q2R simulations of two-dimensional spin glasses

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Abstract. Q2R cellular automata are shown to attain thermal equilibration in the two-dimensional Edwards-Anderson model of a spin glass. Some problems associated with equilibration at low temperatures are identified as finite-size effects. We use a thermalization test due to Bhatt and Young. Our results indicate the possibility of calculating Gibbs averages in this model by means of the Q2R algorithm. A rough efficiency comparison with the conventional (Metropolis) Monte Carlo algorithm is also made.

1. Introduction

Cellular automata are discrete dynamic systems with simple evolution rules that have been proposed as a numerically efficient alternative for the simulation of some physical systems.

In Q2R (Pomeau 1984), binary variables ($S_i = \pm 1$) are located on the sites of a square lattice and they are flipped whenever the sum of its nearest neighbours is zero, so the energy $E = -J \Sigma S_i S_j$ is conserved by this dynamics, making this automaton a possible candidate for the stimulation of the Ising ferromagnet in the microcanonical (μC) ensemble.

This algorithm can be implemented in multispin coding (MSC) using few logical operations and with no need for random numbers, so it is considerably faster than the usual Monte Carlo (MC) method, which simulates the canonical ensemble. Unfortunately, it is highly non-ergodic due to the fact that each spin configuration belongs to a cycle, so after a certain period the starting phase space point will be revisited.

Q2R also shows a cluster period transition (Herrmann *et al* 1987) at $E_{cpt} \simeq -1.75N$, separating two phases with different dynamic behaviours. For $E < E_{cpt}$ there is a fraction of the spins that do not evolve in time. The 'dynamic' sites are located on compact, isolated clusters, embedded in a sea of fixed spins. In this phase the site periods are finite. For $E > E_{cpt}$ the dynamics propagates to the whole lattice and the site periods grow with the system size. Despite this fact, the Ising ferromagnetic transition, signalled by the appearance of a non-zero magnetization $m = \langle S_i \rangle$ and a divergent susceptibility $\chi = \partial m / \partial h$ at $E_c = -\sqrt{2}$ is well reproduced by this algorithm (Herrmann 1986, Moukarzel and Parga 1989) with the sole condition of taking an average over cycles. Other quantities, such as the local energy distribution that can be tested by means of a temperature measurement (Lang and Stauffer 1987), are affected by the non-ergodicity and only give correct results when μC configurations are taken as starting points for the simulation (Moukarzel 1989).

Concerning the numerical efficiency of this algorithm, it has been shown (Zabolitzky and Herrmann 1988) to need, at $T = T_c$, roughly 10 times more updates than the MC

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algorithm in order to travel the same distance in phase space, but even taking this into account, Q2R still wins by a factor two with the codes used by Zabolitzky and Herrmann. Notwithstanding this fact, the capabilities of this algorithm for simulations have not been thoroughly explored, and the attention was mostly centred on its dynamic properties (Stauffer 1990, Stanley *et al* 1987, Costa and Herrmann 1987, Herrmann *et al* 1987). All this refers to the homogeneous Q2R where J is a constant.

Nothing is known about the performance of Q2R for μC simulations of spin glasses, i.e. magnetic systems such that the couplings J are not constant but quenched random variables, chosen with a given distribution (Binder and Young 1986).

In principle, there are reasons to doubt about the usefulness of this μC algorithm to simulate spin glass systems. This is so not only because of the ergodicity problems of this automaton but also because of the existence of a complicated free energy landscape in the spin glass.

However, as we shall show, the ergodicity problems are less severe than in the purely ferromagnetic case. In fact, the fraction of sites that remain frozen after many steps of the ferromagnet Q2R dynamics drops to zero only above and energy threshold, which goes to zero when the system size is increased, as in bootstrap percolation (Stauffer 1990). This phenomenon does not occur in spin glass Q2R where that fraction becomes zero at all energies (except for the ground state energy). This property suggests the existence of large cycles at almost all energies in the spin glass case. This in turn might imply that given a non-typical initial configuration the system will equilibrate, reaching, somewhere along the cycles, configurations that are typical at the energy considered. These would give an adequate sampling to evaluate μC averages.

To avoid the difficulties implied by the rough free energy landscape of spin glass models we studied Gibbs-averaged quantities. This does not represent a limitation since, as is well known, even quantities that are defined in terms of pure states can be evaluated by means of a Gibbs ensemble. For example, the overlap distribution of pure states has its moments given by Gibbs-averaged spin correlation functions (Mezard *et al* 1987). For a canonical simulation this implies taking the large-time limit before the thermodynamic limit. For the Q2R dynamics it means that one should add the contributions of as many equilibrated cycles as possible, obtained from independent initial configurations.

From the above discussion we see that the viability of Q2R μC simulations depends crucially on how well thermal equilibrium is achieved in the largest cycles. The purpose of this paper is to show that for a large enough system such equilibrium indeed occurs.

The specific spin glass system we chose to analyse is the 2D Edwards–Anderson (EA) model (Edwards and Anderson 1975, Binder and Young 1986). For this model there is a single paramagnetic pure state at all finite temperatures; however, the existence of metastable states separated by finite free energy barriers gives rise to freezing effects that make the thermalization of the system difficult (Morgenstern and Binder 1980). The technique we used to prove that this 2D spin glass Q2R thermalizes is an adaptation of the one proposed by Bhatt and Young (Bhatt and Young 1985, 1988a) for canonical simulations. Two different correlation functions that should become equal once equilibrium is attained are defined. As will be emphasized later, these correlations themselves are affected by important finite-size effects and, consequently, their numerical values cannot be compared directly with the canonical ones. But, as we said before, it is only the possibility of reaching equilibrium that we want to explore here.

In the next section the 2D EA model and the Bhatt and Young thermalization test are briefly reviewed. In section 3 the implementation to the spin glass Q2R cellular

automata is discussed. Results are presented in section 4. The last section contains our conclusions.

2. The EA model and the equilibration test

The $\pm J$ EA model of a spin glass (Binder and Young 1986) is characterized by the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J^{ij} S_i S_j \tag{1}$$

with $J^{ij} = \pm 1$, quenched random variables drawn from $P(J) = x\delta(J+1) + (1-x)\delta(J-1)$. We will only discuss the $x = \frac{1}{2}$ case.

The competition between ferromagnetic ($J = 1$) and antiferromagnetic ($J = -1$) ordering gives rise to *frustration* (Toulouse 1977). A plaquette is said to be *frustrated* if it has an odd number of negative couplings. A frustrated plaquette can never have all its bonds simultaneously satisfied. The ground state of the system is highly degenerate due to the existence of zero-energy clusters that can be inverted with no net cost of energy. In two dimensions there is no phase transition at finite temperature because the size of these zero-energy clusters is finite (Morgenstern and Horner 1982) and then the system, no matter how big, can be reversed by finite-energy excitations. The local order parameter $q_{EA} = N^{-1} \Sigma \langle S_i \rangle^2$ must then be always zero in equilibrium because $\langle S_i \rangle = 0$. Nevertheless, the topography of phase space is still complex. There are many low-energy valleys separated by finite free-energy barriers. Different valleys are related by the inversion of some of these zero-energy clusters. In single-flip dynamics, this inversion process takes a time that can be estimated as $\tau \simeq e^{\beta \Delta F}$, with ΔF the free energy barrier the system has to overcome in order to jump from one valley to another. This τ grows rapidly at low temperatures, so in not too long simulations the system remains confined in one such valley and mimics the effect of a spin glass transition at $Tf \simeq 1.0$. It took some time to realize that no transition was really there but, rather, a dynamic effect called 'freezing', due to the fact that relaxation times grow beyond the observation time (but do not diverge as in a real phase transition).

In three dimensions a real spin glass transition is believed to exist (Bray and Moore 1984, 1985, 1987; Bhatt and Young 1985, 1988a, Ogielsky and Morgenstern 1985), but some controversy still remains (Fisher and Huse 1986, Huse and Fisher 1987, Caracciolo *et al* 1990, Reger *et al* 1990) about the relevance that the mean field theory results (Mezard *et al* 1987) may have in finite dimensions, mainly concerning the existence or not of a multiplicity of pure states.

Spin glasses are characterized by their slow dynamics due to the existence of a wide range of relaxation times, so the number of equilibration sweeps needed in a simulation is not easily determined in these systems. In fact, this number is not even uniquely defined, because different magnitudes take different times to equilibrate. Nevertheless, one could estimate such a thermalization time from, for example, the equilibration of the order parameter distribution $P(q)$. Bhatt and Young (1985, 1988a) have proposed a method to estimate this time, which we now briefly discuss.

First define the autocorrelation overlap as

$$q_a(t_0, t) = \frac{1}{N} \sum_i S_i(t_0) S_i(t_0 + t) \tag{2}$$

where t is the number of lattice updates separating both configurations and t_0 is an equilibration time. The interesting quantity is the probability distribution

$$P_a(q, t_0) = \frac{1}{\tau}\left[\sum_{t=t_0+1}^{t_0+\tau} \delta(q - q_a(t_0, t))\right]_{av} \tag{3}$$

where τ ($\tau \ll t_0$) is the number of times that the autocorrelation overlap is recorded, so the mean separation between configurations is approximately t_0, and $[\ldots]_{av}$ denotes an average over bond samples.

The overlap between replicas is defined as the projection of two independent copies of the system, with the same realization of couplings

$$q_r^{12}(t_0) = \frac{1}{N}\sum_i S_i^1(t_0) S_i^2(t_0) \tag{4}$$

and the distribution of this magnitude is calculated as

$$P_r(q, t_0) = \frac{1}{\tau}\left[\sum_{t=t_0}^{t_0+\tau} \delta(q - q_r^{12}(t))\right]_{av}. \tag{5}$$

The dimensionless ratio g is a ratio between moments of $P(q)$, which will be useful to follow the equilibration process

$$g = \frac{1}{2}\left(3 - \frac{\langle q^4\rangle}{\langle q^2\rangle^2}\right). \tag{6}$$

Suppose we calculate g_a and g_r (from $P_a(q)$ and $P_r(q)$, respectively) as a function of t_0. For early times the autocorrelation overlap will be approximately one so $P_a(q)$ will be highly peaked as $q \simeq 1$ and g_a will be near to one. On the other hand, if the replicas are started from independent random points in phase space, they will be initially decorrelated, so $P_r(q)$ will have the form of a Gaussian centred at $q = 0$ and $g_r \simeq 0$.

The dynamics of the system will push the replicas to certain regions of phase space, so, in the limit of $t_0 \to \infty$, $P_r(q)$ will be the equilibrium distributuon $P(q)$, and so will $P_a(q)$ in the same limit because two configurations can be regarded as independent when they are separated by a long time. We see then that g_a will *decrease* and g_r will *rise* towards the equilibrium value, but starting from opposite sides.

As we shall see later on, the possibility that g_r or g_a is non-monotonous cannot be ruled out, so that, if at a certain time we have almost convergence of the two, nothing ensures that the equilibrium value will lie between them. For the models reported (Bhatt and Young 1985, 1988a, b, Reger *et al* 1990) g_a decreased and g_r increased steadily in time till they met at the (temperature dependent) equilibrium value, and then they continued to agree (although the possibility that g behaved in a non-monotonous way was pointed out by the authors). In those cases when both values coincide the system can be regarded as equilibrated.

3. The spin glass Q2R: its numerical implementation

A few details must be discussed before applying this method to test thermalization in Q2R. First, we have to define how we will relate the μC and canonical ensembles. Following standard statistical mechanics arguments, we expect μC averages at energy E to coincide with canonical ones at temperature β^{-1} such that $\langle H\rangle_\beta = E$. This suffices to establish the link between ensembles in the case of homogeneous systems, but in

disordered models $E(\beta)$ depends on the sample, and might also be in the valley. In this case we have to specify a prescription to relate MC and Q2R simulations to each other.

The valley dependence is not important as long as one is simulating finite systems so, in practice, just one pure state exists, and we can define $E_s(\beta)$ uniquely for a given sample s as its Gibbs-averaged energy.

The sample dependence is somewhat more delicate. What one should do to be rigorous is to perform the Q2R simulations at energies that depend on the sample one is considering, so as to make them correspond to the same temperature. In this way one can safely average over samples. This would require complex programming and a previous MC simulation on each sample that one was to use in Q2R. What we do instead is to define a sample-averaged $E(\beta) = [E_s(\beta)]_{av}$ and make all Q2R simulations at the same energy (for a fixed equivalent temperature). This approach is supported by the self-averageness of E and should be correct for large enough systems.

The other point concerns the construction of the starting states for Q2R simulations. While in MC simulations the temperature is an external parameter, in μC simulations the control parameter is the energy, which is configuration dependent, so we have to define a method to obtain starting states of a given energy.

Different methods could yield different results. To see this, think of the extreme case where our states had exactly μC distribution. Then the distribution of overlaps between replicas would be the equilibrium one and there would be nothing to equilibrate. This would be the case if we used the starting states described by Moukarzel (1989), but that method is of no practical use in this case, due to the time needed to equilibrate a spin glass.

The method we used was the following. First, all the replicas were initialized in random configurations. As a result their energy was very high. Afterwards their sites were visited at random and the spins flipped whenever the energy did not rise, until the desired value was reached. If, after 300*N of these spin flip trials, any of the replicas did not reach the desired energy, then the whole sample was discarded and a new set of bonds was constructed.

A different strategy like, for example, repeating the previous procedure a certain number of times before discarding the sample could have been used, but we chose this one for ease of programming. It has the drawback of biasing the sampling. Bond sets whose low-lying states are not easily reached have less probability to be accepted for a simulation at low energy. Anyway, we found that this point is not important for large lattices (the sample rejection rates were 0, 0, 10%, 60% for $L = 16$ at $T = 1.2$, 1.1, 1.0, 0.9 and 0, 0, 0, 5% for $L = 32$ at the same temperatures).

To test thermalization we ran three independent spin configurations (replicas) for each sample. This number was chosen in order to have the same statistics for q_r and q_a. First the replicas were updated t_0 times. Then their mutual overlaps q_r were recorded during 100 more steps, storing the configurations after each Q2R step. Afterwards we continued updating without further measurements up to $t = 2t_0$. During the following 100 steps, each of the replicas was projected on the corresponding stored configuration, so obtaining the overlaps q_a between configurations separated by exactly t_0 steps. In this way, and after averaging over samples, we obtain $P_r(q)$ and $P_a(q)$ for a given time t_0.

The average was done over 400–500 samples. The data were accumulated in four statistically independent groups. Error bars in the figures indicate the error estimates from the dispersion of the four groups.

4. Results

4.1. Frozen sites

The frozen sites at a given time t are those that have not changed their state since the beginning of the simulation. This magnitude is useful for determining whether the dynamics spreads to the whole lattice or remains confined, at a given energy. It is somehow related to the existence of a cluster period transition.

We have measured the frozen fraction Fz for several energies and times for the ferromagnet and the spin glass. At each energy, Fz was averaged over 50 different starting configurations. The spin glass initial states were constructed from one ground state of a unique sample, obtained by careful annealing. No sample average was done in this case.

In figure 1 we can see Fz versus energy for the ferromagnet and the spin glass. Each curve corresponds to a different observation time. For the ferromagnet, an energy threshold can be seen to exist below which the dynamics does not spread to the whole lattice. This threshold has been shown to be size dependent (Stauffer 1990). Looking at figure 1 one can estimate its location somewhere between $E=-1.7$ and -1.6, for $L=64$. The spin glass behaviour is different. In this case the threshold seems to be the ground state itself. In temperature terms, the spreading threshold is located at $T=0$ in the spin glass and at a finite temperature in the ferromagnet.

This suggests that a cluster period transition could only exist at $T=0$ in the spin glass Q2R. This would constitute an advantage of the spin glass case from the point of view of ergodicity.

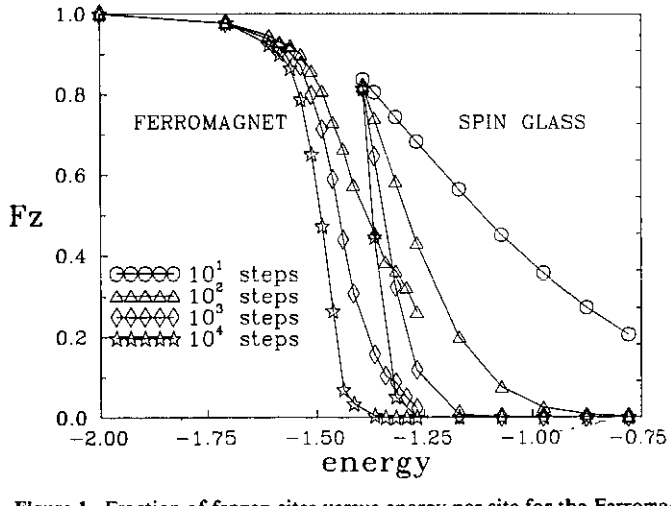

Figure 1. Fraction of frozen sites versus energy per site for the Ferromagnet Q2R and spin glass Q2R for different observation times. These values are for an $L=64$ lattice.

4.2. Temperature measurement

The temperature can be determined (Lang and Stauffer 1987, Moukarzel 1989) in the μc ensemble through the local energy distribution, which must satisfy

$$\frac{P(+\varepsilon)}{P(-\varepsilon)} = e^{-2\beta\varepsilon}. \tag{7}$$

We have measured the probability $P(n)$ for a site to have local energy n in spin glass Q2R. From these, two independent measurements of T can be made:

$$T_2 = \left[\frac{1}{4}\log\left(\frac{[P(-2)]_{av}}{[P(+2)]_{av}}\right)\right]^{-1} \tag{8}$$

$$T_4 = \left[\frac{1}{8}\log\left(\frac{[P(-4)]_{av}}{[P(+4)]_{av}}\right)\right]^{-1}. \tag{9}$$

The simulations were made at energies corresponding to $T = 0.9$, 1.0, 1.1 and 1.2. In figure 2 we can see that both estimates coincide with each other after an equilibration time that depends on temperature.

The coincidence between measured T and $T(E)$ is not always good. The differences are not even systematic, so we do not have a clear explanation for this.

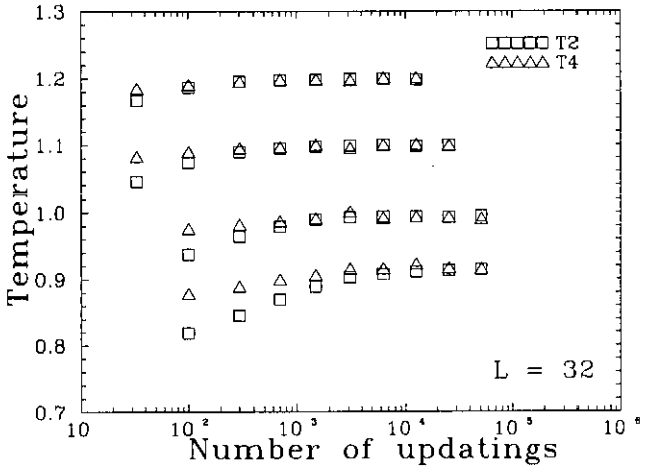

Figure 2. Measured temperatures T_2 and T_4 in spin glass Q2R versus simulation time. Shown are the results obtained for $L = 32$. The Q2R simulations were made at energies corresponding to $T = 0.9$, 1.0, 1.1 and 1.2. These values are instantaneous (not time averaged) so they reflect the time evolution of the local energy distribution.

4.3. Thermalization

For $L = 8$ (figure 3), thermalization is not attained by Q2R but at the highest temperatures. For $L = 16$, Q2R fully thermalizes in less than 10^3 iterations at $T = 1.2$ (figure 4). At low temperatures a crossing between g_a and g_r occurs that will be discussed later. In $L = 32$ (figure 5) the thermalization is complete but, at $T = 0.9$, the lowest temperature we simulated, where a small crossing of gs also appears.

We include MC data for the same sizes and temperatures for comparison purposes. It is seen that MC simulation always thermalizes in less iterations.

The crossing of g's that can be observed for $L = 16$ at low temperatures is due to the appearance, in the 400×3 configurations that were sampled to construct $P_a(q)$, of a few trapped configurations that never go far from the starting point. As a result $P_a(q)$ conserves, for $T = 0.9$ and $T = 1.0$, a small peak near $q = 0.8$ (figure 6) due to configurations that, after many updatings, are still near the starting point.

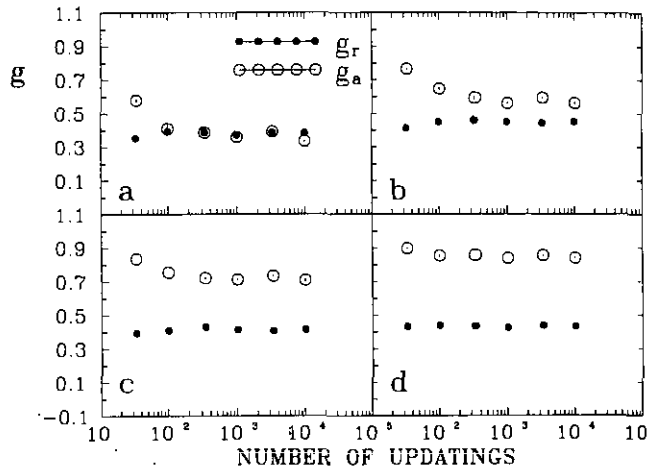

Figure 3. Dimensionless ratio g for Q2R in $L = 8$ spin glass versus time. The (approximate) equivalent temperatures are: (*a*) $T = 0.97$, (*b*) $T = 1.07$, (*c*) $T = 1.17$ and (*d*) $T = 1.4$. An average was made over 480 samples at each temperature.

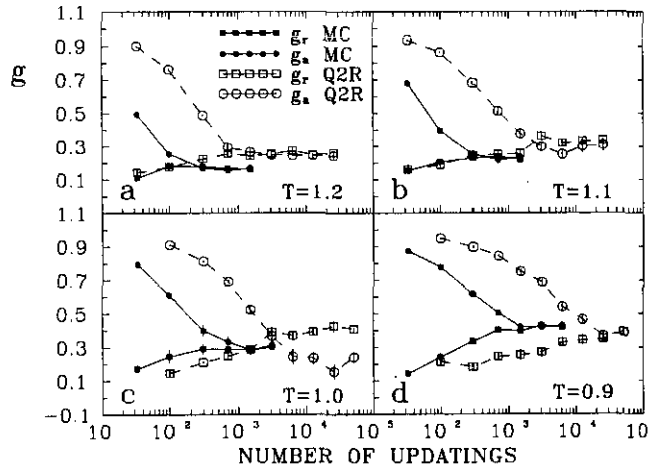

Figure 4. Dimensionless ratio g for Q2R and MC algorithms versus time for $L = 16$ in the spin glass.

Surprisingly this peak *does not raise* the ratio g_a but *lowers* it. This is unexpected because one knows that a distribution concentrated around $q = 0.8$ will have $g \simeq 1$ and another centred at $q = 0$ will have $q \simeq 0$, so one intuitively expects that a superposition of both will have a ratio g somewhere between 0 and 1. In fact, this is not true. It can be shown that if one adds two Gaussians, one centred at $q = 0$ with weight $(1-\varepsilon)$, and the other at Q_p with weight ε, the ratio g for this combined distribution may be negative for intermediate values of ε, while being zero for $\varepsilon = 0$ and almost one for $\varepsilon = 1$ (figure 7).

We have also verified that, within this two-Gaussian approximation, the crossing is well reproduced if the Gaussians are chosen so as to approximate the case of $T = 1.0$ and $L = 16$ (figure 6), for appropriate peak weight ε and peak position Q_p.

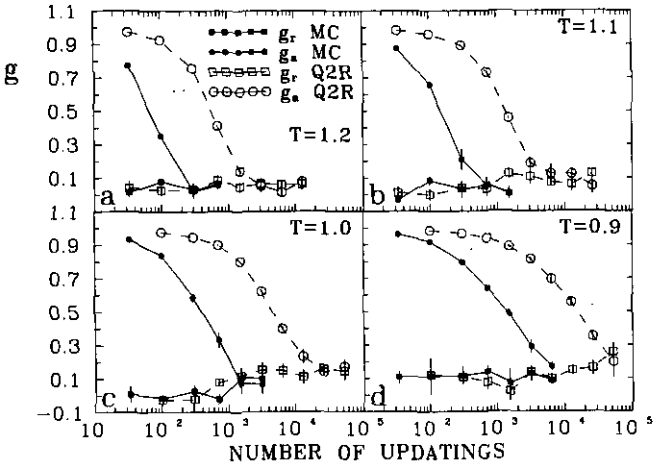

Figure 5. The same as figure 4 for $L = 32$.

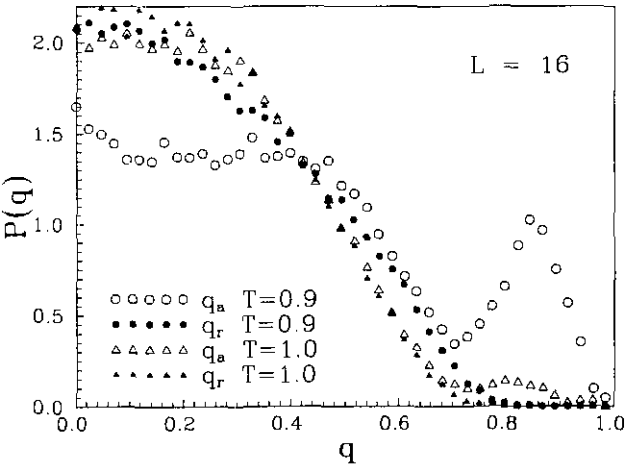

Figure 6. Distribution $P(q)$ of autocorrelation (q_a) and replica (q_r) overlaps for $L = 16$ at the longest times simulated in $T = 0.9$ and $T = 1.0$. The peaks of trapped configurations appear in $P(q_a)$ at $q \simeq 0.8$.

For $L = 16$ and $T = 0.9$, these trapped configurations lower the value of g_a, making it similar to g_r. This results in the corresponding g graph (figure 4(d)), which suggests that thermalization has been attained, although looking at the corresponding $P(q)$ (figure 6) we see this not to be true. Indeed, thermalization is worse in this case than for $T = 1.0$. For $L = 32$ we verified that no peak of trapped configurations appeared at $T = 1.2$, 1.1 and 1.0 (figure 8). For this size the coincidence of g_a and g_r was accompanied by a coincidence of $P_a(q)$ and $P_r(q)$ within errors. A very small peak ($\varepsilon \simeq 8 \times 10^{-4}$) shows up in $P_a(q)$ for $L = 32$, $T = 0.9$, for $t_0 = 5.1 \times 10^4$. In this case the values of g_a and g_r could again be interpreted as suggesting full equilibration while $P(q)$ clearly shows (figure 8(d)) that ethis is not true yet.

As mentioned earlier, the convergence of g_a and g_r may not be a safe indicator for thermalization.

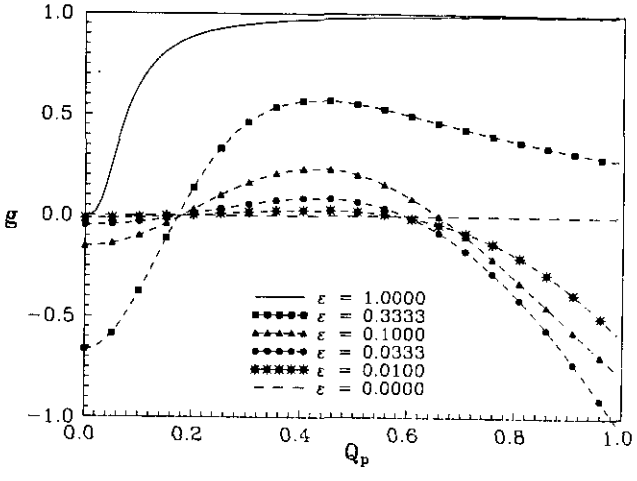

Figure 7. Dimensionless ratio g for a superposition of two Gaussians. The first one has dispersion 1, weight $(1-\varepsilon)$ and is centred at 0 while the second has dispersion 0.1, weight ε and is centred at Q_p. Shown is g very Q_p for several values of ε. Note that for certain values of Q_p, $g(\varepsilon)$ is non-monotonous.

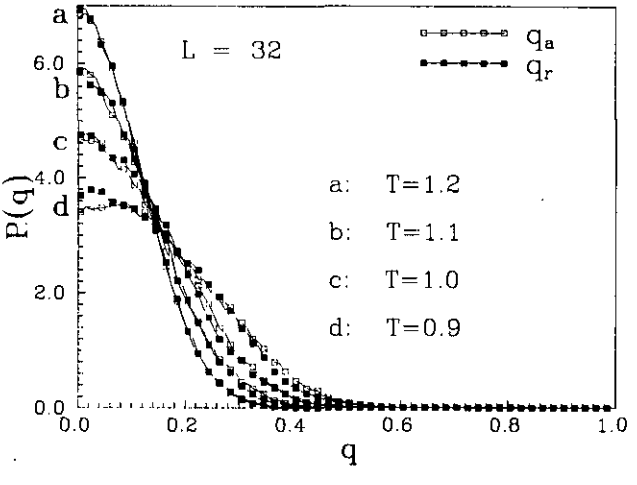

Figure 8. Distribution $P(q)$ of autocorrelation (q_a) and replica (q_r) overlaps for $L=32$ at the longest times simulated in $T=1.2$, 1.1, 1.0 and 0.9.

Our data suggest that the inability of Q2R to equilibrate is a finite-size effect, confined to lower temperatures as N is increased (compare figure 6 to figure 8). It is then to be expected that at any finite temperature the 2D spin glass Q2R will attain equilibrium on large enough lattices.

Let us mention that the values of g^{eq} obtained with MC and Q2R simulations do not coincide with each other. This is not a problem since the existence of a non-null g in the 2D EA model at finite temperature is a finite-size effect (Bhatt and Young 1988*a*), and we know that finite-size effects depend strongly on the ensemble. Consequently, coincidence of g_{Q2R} with g_{MC} is not to be expected for finite sizes.

We now turn to the point of the relative efficiency of Q2R and MC algorithms. Both Q2R and MC programs, were implemented in multispin coding. In both cases 32 lattice sites are simultaneously updated.

The MC code performs in a fully parallel fashion, including the comparison with a random number. The code in this case is the one described by Williams and Kalos (1984) with the modifications introduced by Pierre *et al* (1987). These modifications reside in the way in which a string of random bits with probability $e^{-4\beta}$ is constructed from the available random bits with probability $\frac{1}{2}$ ($\frac{1}{2}$ bits). The first method (Williams and Kalos 1984) needs too many $\frac{1}{2}$ bits per site at low temperatures while the second one (Pierre *et al* 1987) performs with a (fluctuating) number of bits per site that is roughly temperature independent and approximately 7 (for a 32 bits word) on the average. A shift register with the pair (521, 32) was used as a random-number generator (Kirkpatrick and Stoll 1981).

The Q2R code (Herrmann 1986) is similar to the MC one, but the decision of flipping a spin requires less operations because no random numbers are needed and also because only sites with zero local field need to be identified. With this arrangement, the relative efficiency per Q2R and MC sweep gives an approximate factor of five in favour of the former.

By looking at the g-graphs one can make some very rough estimates of the number of lattice sweeps (t_{MC}^{eq}, t_{Q2R}^{eq}) needed for equilibration in each case. For $L=16$ we have $(2\times10^2, 9\times10^2)$ at $T=1.2$. For $L=32$ one finds $(3\times10^2, 1.8\times10^3)$ at $T=1.2$, $(5\times10^2, 4\times10^3)$ at $T=1.1$ and $(1.5\times10^2, 1.8\times10^4)$ at $T=1.0$. It is apparent that t_{Q2R}^{eq} grows faster than t_{MC}^{eq} at T is decreased. For $L=32$ the relative factors between them are 6, 8 and 12 at $T=1.2$, 1.1 and 1.0. An analysis of the size dependence of this factors can not be made on the basis of our data.

Taking into account than one MC sweep takes five times more CPU time than a Q2R one, it is found that the MC algorithm is always more efficient for equilibration at the temperatures we have simulated. An extrapolation to higher temperatures suggests that Q2R could be globally more efficient for $T \geqslant 1.3$.

5. Conclusions

We have shown that the microcanonical algorithm Q2R is able to attain equilibrium in the case of a 2D EA model of spin glasses with nearest-neighbours interactions ±1. This is not at all obvious since the non-ergodic characteristics of Q2R in the case of the ferromagnet are well known (Herrmann *et al* 1987, Moukarzel 1989). The multiplicity of ergodic phases is also a characteristic of spin glasses (but certainly with a different origin: in the case of Q2R it is a property of a dynamics while in the case of spin glasses it stems from the characteristics of the free energy surface of the model) so, in principle, one could expect that a combination of both would not work. The result is then that non-ergodicities do not add up in this case.

We have found here an example where the behaviour of g is non-monotonous. The same would happen for any dynamics that produced a $P_a(q)$ with a two-peak structure at intermediate times before thermalization. This might be produced, for example, if most configurations decorrelate in a given number t_1 of iterations but a certain fraction ε of them take a longer time, $t_2 \gg t_1$. For $t_1 < t < t_2$, $P_a(q)$ would have this two-peak structure, which could produce the effects we have described.

All the numbers concerning equilibration times in this work have to regarded as rough estimates. A more precise analysis of this point as well as of its dependence on system size would be worthwhile, but it requires much more statistics.

A similar analysis would be needed in the interesting case of the three or more dimensional EA model where a finite temperature phase transition is believed to occur. Also, a multiplicity of pure states might be present in this case, and it is not known how these facts will affect the ergodicity of Q2R.

From the point of view of numerical efficiency, let us note that multispin-coded MC needs, in three dimensions, twice as many random numbers per site as it does in two dimensions, while the (per site) computational efford needed in Q2R is almost the same in two and three dimensions (just a few more logical operations are needed to identify the zero-field sites).

About 1500 CPU hours on a MicroVAX-II were used in this work.

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