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Cellular automata as microcanonical simulators

Paulo Murilo C de Oliveira, Thadeu J P Penna, Suzana M Moss de Oliveira and Rita Maria Zorzenon

Instituto de Física, Universidade Federal Fluminense, Caixa Postal 100296, Niterói, Rio de Janeiro, Brazil 24000

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Abstract. The deterministic Q2R cellular automaton has been tested by many authors as a fast algorithm to simulate the Ising model in the microcanonical ensemble. However, the magnetic susceptibility curve, measured from the fluctuations of the magnetization, is found to be far below the expected results inside the ordered Ising phase. The non-ergodicity degree of this automaton seems to be inadequate to simulate the Ising dynamics. In this work, we introduce two modified automata, and test their performance for the square lattice. For the first one, we found improved results concerning the Ising transition. For our second modified automaton the Ising transition does not occur, the magnetization vanishing even for energies far below the normal critical threshold. On the other hand, another transition appears at a different critical energy value that seems to be the same as that of the periodic–chaotic transition already observed in the normal Q2R dynamics. The critical indices of this new transition are measured from finite-size scaling, the results indicating that it is at the same universality class as the Ising transition.

1. Introduction

The idea of using deterministic cellular automata (CA) to simulate statistical models was first proposed by Pomeau [1] and Vichniac [2], exploring the parallel processing characteristic of CA and the absence of random numbers in order to obtain fast simulations. For the square lattice ferromagnetic Ising model, the local energy e stored in the four bonds linking each spin to its neighbours can assume values 0, 1, 2, 3 and 4, according to the number of these neighbours presenting opposed spins relative to the central one. The total energy is

$$E = \sum_{\langle ij \rangle} \sigma_i \otimes \sigma_j \tag{1}$$

where the sum covers the nearest-neighbour pairs of sites, σ_k is a Boolean (0 or 1) variable representing the current spin up or down at site k, and $\otimes$ represents the XOR (eXclusive OR) logical operation. Equation (1) simply defines the energy as the current number of broken bonds in the lattice, i.e. the number of pairs of neighbouring sites presenting opposed spins.

The most common way to simulate the thermodynamic behaviour of this model is the so-called Metropolis algorithm [3]. In this case, one tests the local energy of each spin. If it is 2, 3 or 4, the spin is flipped, transforming the local energy to 2, 1 or 0, respectively. This recipe corresponds to the relaxation step, allowing the system to release energy to the environment. If the local energy is 1 or 0 the flipping is also allowed, but now according to probabilities $\exp(-2/T)$ and $\exp(-4/T)$, respectively.

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This second stochastic fluctuation step allows the system to absorb energy from an environment maintained at a constant temperature T, and guarantees that states iteratively generated by this rule appear with a frequency proportional to the Boltzmann factor $\exp(-E/T)$ corresponding to the canonical ensemble. The thermodynamical average $\langle Q \rangle$ of some quantity Q is obtained simply by summing the values of Q corresponding to a sequence of states generated by the above recipes, discarding a certain quantity of the initial states in order to avoid influences of the artificially chosen initial state (the so-called thermalization transient).

One of the main problems concerning simulations is the computer time consumption. In order to overcome this problem and improve the performance, a multi-spin code [4] was introduced. In this code, many non-nearest-neighbour spins are updated simultaneously, using the fast bitwise parallel operations AND, OR, XOR, NOT and SHIFT provided by any digital computer. For the square or cubic lattice Ising model, the spin and the local energy of each site are stored in just four bits of a computer word. On 16-bit personal computers, for instance, this strategy allows the storage of four spins in only one computer word, updating the system in parallel for sets of four spins simultaneously. In the case of 64-bit mainframes, sets of 16 spins are treated in parallel.

In an improved version [5] only the spin states are kept, there being no need to store the local energy values. Storing one spin state per bit, the number of spins updated simultaneously in parallel is the same as the computer word length (16 on PC). The square lattice, for instance, must be divided in two chessboard sublattices, the updating being performed first for one of them and then for the other one. Other lattices must also be divided in a similar way, with no nearest-neighbour spins in the same sublattice. However, in all those references the stochastic step is performed *sequentially* by generating a real random number between 0 and 1 and comparing it with the relative Boltzmann factor $\exp(-2/T)$ or $\exp(-4/T)$ corresponding to local energies $e = 1$ or 0, in order to decide if the spin must or must not be flipped. This procedure consumes much computer time, compromising the efficiency of the simulations. In order to improve the performance of such simulations, instead of random real numbers, another improved version [6] uses words whose bits randomly assume the value 1 according to a predefined probability which can be adjusted to coincide with $\exp(-2/T)$ or $\exp(-4/T)$, allowing the completely parallel treatment of the problem.

The CA alternative was introduced to bypass the stochastic step. For the square lattice, the Q2R rule corresponds simply to flipping the spin if and only if the corresponding local energy is $e = 2$. Again, the lattice must be divided into two chessboard sublattices. This rule does not alter the energy of the system, and for this reason it is supposed to perform a microcanonical simulation of the Ising model [1, 2]. The question about the adequate spanning of the space of states in this automaton, as compared with the correct Ising dynamics, however, remains to be answered. Supposing, for the moment, that we are dealing with a true microcanonical simulator, let us analyse how to measure thermal averages. Contrary to the canonical ensemble, where the energy E fluctuates and a constant-temperature thermal average $\langle E \rangle$ must be measured, in microcanonical simulation the value of E itself is maintained constant. Both ensembles are rigorously equivalent, and thermal averages can also be obtained from microcanonical simulations. In this case, one must obtain the temperature T for which the canonical averaged energy $\langle E \rangle$ would coincide with the constant value E adopted in the real microcanonical simulation. One way to do this was proposed by Lang and Stauffer [7] through the probability $P(e)$ of obtaining local energy e at a

given site. For instance, consider one site with $e=1$. By flipping this spin, maintaining all others in their current states, the increment in the energy would be 2, and the local energy would change to $e=3$. The Boltzmann factor corresponding to the whole system would be also decreased by a factor $\exp(-2/T)$. Thus, one can use the relation

$$\frac{P(1)}{P(3)}=\exp(2/T) \tag{2a}$$

in order to determine the value of T from $P(1)$ and $P(3)$, both measured from a microcanonical simulation. Analogously, one can measure $P(0)$ and $P(4)$, obtaining the temperature T from

$$\frac{P(0)}{P(4)}=\exp(4/T). \tag{2b}$$

The energy-dependent microcanonical average $\langle Q\rangle$ of some quantity Q can be plotted as a function of T instead of E, by using the relation $T(E)$ obtained from the same simulations through equation (2*a*) or (2*b*).

Concerning the computational performance, the advantage of this strategy over the Monte Carlo alternative is the absence of random numbers and comparisons. The computer time consumption is drastically reduced for each update of the whole system, although more updates are needed in order to obtain good averages. Comparing the performances obtained for the canonical Monte Carlo simulations using the completely parallel code [6] and for the Q2R code [8] that is also completely parallel, both running on the same 16-bit computer, we conclude that there is no real advantage in using Q2R, because the time saving obtained due to the faster update of the whole lattice does not compensate the need of a greater number of updates. The same behaviour must also be expected for vectorized computers, as the same vectorization tricks [9] can also be applied to the completely parallel Monte Carlo code [6], which uses exactly the same storage and updating strategy.

Nevertheless, the non-ergodicity degree of Q2R, as compared with the true Ising model, is still an open question, and many recent works [7–12] are dedicated to investigating it. For this reason, we think that there are many points to be clarified in the study of Q2R and related CA, in particular their relation to the Ising model (up to now, this relation is not clear at all). The square lattice magnetization was measured for large lattices (up to 1280×1280) [8], and the results are in complete agreement with the exactly known Onsager solution. For the cubic lattice, Lang and Stauffer [7] also found good agreement with available Monte Carlo data for the magnetization and specific heat above and below the critical point, as well as for the susceptibility only above the critical point. They also compared Q2R data for the magnetization fluctuations to the susceptibility curve obtained from Monte Carlo canonical simulations below the critical point: discrepancies of up to two orders of magnitude are observed, indicating that the Q2R rule should underestimate the real fluctuations of the true Ising dynamics in the ferromagnetic phase. Later, Moukarzel and Parga [10] realized that microcanonical fluctuations cannot be directly compared to the susceptibility curve, without the inclusion of a correcting term accounting for the canonical energy fluctuations absent from the microcanonical scheme. However, even after the inclusion of this correction, Q2R data for the square lattice are still below the expected curve.

Another interesting point is the influence of the starting spin state. In order to simulate some energy value E, one must first choose a convenient initial distribution of spins up and down along the lattice, the resulting energy coinciding with the desired

value E. Starting from the ferromagnetic ground state (all spins up), flipping spins one after another at random, and measuring the energy after each flip until the desired value is reached, one succeeds in constructing such an initial state [7, 10, 11]. We always used this procedure in the present work. In this case, as observed by Moukarzel [11], the relative distributions $P(e)$ of sites with local energies ($e=0$, 1, 2, 3 and 4) does not match the corresponding distributions observed in thermalized states obtained from Monte Carlo canonical simulations, even after many Q2R updates are performed. Deviations between the curves $T(E)$ obtained from equations (2*a*) or (2*b*) and the correct curve [13] are observed [11] below the critical point. On the other hand, starting from previously thermalized states presenting the correct relative distributions $P(e)$, obtained from canonical Monte Carlo simulations, the correct curve $T(E)$ was successfully reproduced by the Q2R dynamics [11]. This fact shows that Q2R dynamics is not able to mix adequately all the possible different relative distributions of local energies, in order to reach the equilibrium ratios (2*a*) and (2*b*). The important conclusion is that the non-ergodicity degree of Q2R is really not adequate to simulate the Ising model below the critical point. Although the Q2R dynamics breaks the symmetry at the right critical energy spanning only one half space of states below it (the positive magnetization half, for instance) giving rise to a phase transition, it does not span this half space adequately, underestimating the degree of fluctuations characteristic of the ferromagnetic Ising phase. Actually, even above the critical point, Q2R dynamics is known to be non-ergodic [14]. Although the true Ising dynamics must also be non-ergodic, in order to give the correct averages for the various thermodynamic quantities and to break the symmetry between positive and negative magnetizations below the critical point, the degrees of non-ergodicity are distinct for these two dynamics.

A third interesting point about Q2R is that, besides the Ising-like transition occurring at the critical energy density $\mathscr{E}_c=(2-\sqrt{2})/4=0.146$, it presents a second transition [12] at another lower critical value $\mathscr{E}_p\approx 0.063$ (estimated for 64×64 finite lattices, in reference [12]). Below this value, the dynamic evolution of each spin has a finite period (much less than 2^N, where N is the number of sites in the lattice), while infinite periods (of the same order of 2^N) were found above this threshold. The name 'periodic-chaotic' [12] will be used hereafter to refer to this transition. Compact clusters of neighbouring spins oscillate with the same period below $\mathscr{E}_p$, and the closer the energy to this threshold, the larger the mean cluster size. The second moment of the cluster period distribution presents the same behaviour as the susceptibility of a normal magnetic transition, blowing up at $\mathscr{E}_p$. Up to now, the physical mechanism responsible for this transition has not been fully understood.

Some recent works on Q2R dynamics [15, 16] show that a very large number of time steps are needed in order to improve the numerical results for thermal averages. Nevertheless, as inferred from the above discussion, the Q2R dynamic rule does not adequately span the half space of states corresponding to positive magnetization, and cannot be considered as a good microcanonical simulator for the Ising model below the critical energy threshold. The aim of this work is to introduce some modified CA rules in order to improve the mixing capacity of the corresponding dynamics. Two of these modified rules [17, 18] are presented and discussed. For details about the computation strategy, see [19]. Adopting the first modified rule, we are able to obtain good numerical results for both the magnetization and susceptibility, although taking only a reasonable number of time steps. The second modified rule presents another unknown transition which is studied through finite-size scaling.

2. First modification

Instead of considering only the four bonds linking each site to its four nearest neighbours, we will now take into account the six bonds linking each pair of nearest-neighbour sites to its surrounding neighbourhood, as shown in figure 1. Maintaining fixed the six spins around the central pair of sites linked by the thick dark line, both spins will be flipped if this change does not alter the energy of the system, i.e. if just three among the six neighbouring bonds are currently broken. The energy quanta stored in these broken bonds now have a greater mobility along the lattice, during the dynamic evolution. Our idea is that this increased mobility can also enhance the degree of ergodicity in the space of states, improving the results obtained from the simulation.

Now, the parallel processing cannot be performed for one entire chessboard sublattice simultaneously, but another geometric division of the lattice is necessary, as shown in figure 2. The pairs corresponding to the thick dark lines are updated in parallel for the left figure, then the same process is repeated for the right figure, and again for six similar geometric arrangements. After the whole process, each spin is updated four times, as it has four nearest neighbours, belonging alternately to four different thick dark lines during the dynamic evolution. We used periodic boundary conditions.

We performed simulations for 128×128 lattices, taking ten different starting states for each energy value. Figures 3 and 4 show the averaged values for the magnetization and its fluctuation, respectively. Full curves correspond to the exact solution of the

Figure 1. Two distinct schemes for the dynamic rules proposed to simulate the square lattice Ising model in the microcanonical ensemble. In Q2R (left), the central spin is flipped if just two of the four bonds linking it to the neighbourhood are currently broken (opposed spins). In our proposal (right), both spins linked by the thick dark line are flipped if just three among the six bonds linking them to the neighbourhood are currently broken.

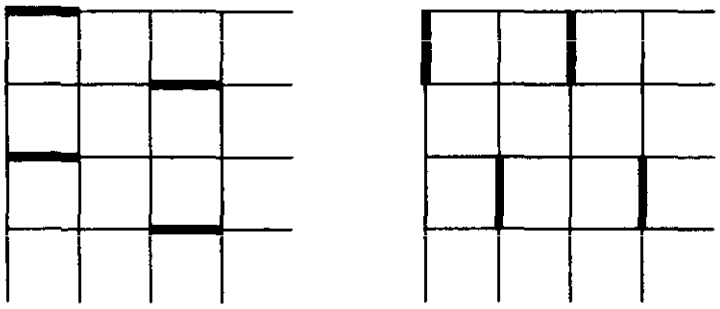

Figure 2. Scheme of the first two parallel updating steps of our modified CA rule. One complete update of the whole lattice corresponds to a total of eight such steps, each spin being updated four times.

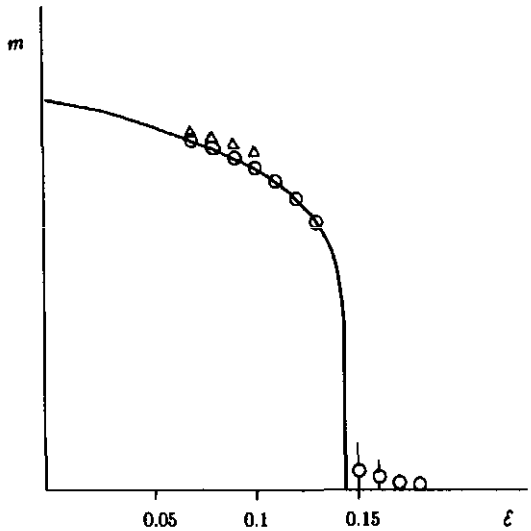

Figure 3. Magnetization as a function of the energy. The full curve is the exactly known curve. Results obtained from Q2R cellular automaton correspond to triangles, while the circles show the values obtained from our first modified dynamic rule.

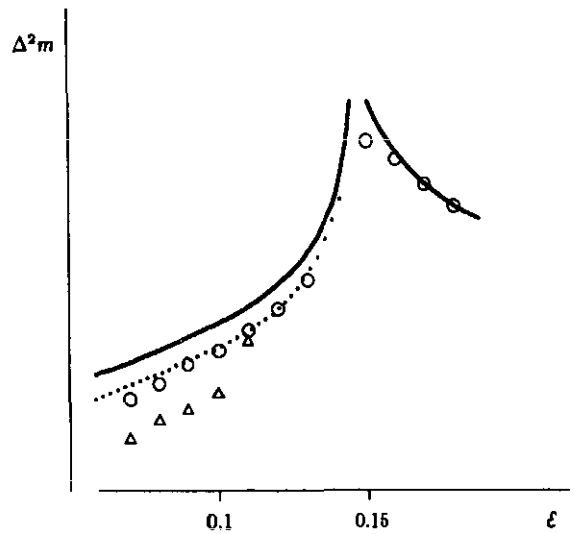

Figure 4. Mean squared fluctuation of the magnetization as a function of the energy. The full curve corresponds to the canonical exactly known result, being equal to the product $T\chi$. The dotted curve corresponds to the microcanonical correction. The vertical scale is logarithmic.

Ising model in the canonical ensemble, the one in figure 4 being equal to the product temperature × susceptibility. The dotted curve corresponds to the microcanonical magnetization fluctuation, and was obtained from Monte Carlo canonical simulations using the correction term defined by Moukarzel and Parga [10]. The number of complete updates for each initial state varied from 10^5 (for $\mathscr{E} = 0.07$ and 0.18) to 10^6-10^7 (for $\mathscr{E} = 0.13$ and 0.15). For $\mathscr{E} = 0.14$, even taking 10^7 updates, we did not succeed in

obtaining reliable numerical results, due to the large fluctuations observed. The computer time for each complete update is one order of magnitude higher than in Q2R. Triangles correspond to Q2R data, while circles show the results obtained from our modified CA. For energies where only circles appear, both values coincide. The error bars are smaller than the symbols, except for two points just above the transition, in figure 3. The maximum observed for $\mathscr{E} \approx 0.15$ in figure 4 agrees with the correct known value for 128×128 lattices. Small deviations are observed for the lower energies ($\mathscr{E} = 0.07$ and 0.08) for our CA, while much larger deviations (the vertical scale is logarithmic) occur since below $\mathscr{E} \approx 0.11$ in the case of Q2R. These deviations also vanish in the case of Q2R, if one takes more and more updates [15, 16]. This very slow relaxation behaviour is nicely demonstrated by measuring the time rate of damage spreading [15].

3. Second modification

Returning to our idea that Q2R is a very restrictive rule concerning the allowed movements of the energy quanta stored in broken bonds, we will now introduce another modification in this CA.

In the previous modified CA defined in section 2, *all* energy quanta are allowed to move up to two lattice parameters in each update, instead of only one lattice parameter allowed in Q2R (see figure 1). Now, we will return to the ordinary Q2R rule. After each complete Q2R update of the whole lattice, however, a complementary update is introduced: we search for a site whose local energy is currently $e = 0$, and also for another site with $e = 4$, flipping both the corresponding spins. The total energy is also conserved. Another Q2R complete update is then performed, followed by another search for two spins with local energies $e = 0$ and 4, and so on alternately. The search for the $e = 0$ site is performed sequentially along the lattice, starting from the location where it was found in the previous step. The same procedure is also used in searching for the $e = 4$ site. As only two more spins are updated than would be by the Q2R traditional rule in each step (for a 512×512 lattice, the largest size we tested, this represents less than 0.001%), one might think that this new CA rule would lead to a negligible change in the results. Nevertheless, the $e = 0$ site can be found at any distance from the corresponding $e = 4$ site, introducing a *non-local* transport of energy that represents a *qualitative* change in comparison with Q2R-like dynamic rules, which allow energy transport in only small scales of length.

Simulations performed for 64×64 finite lattices show that the Ising transition at $\mathscr{E}_c = 0.146$ disappears. A vanishing magnetization was measured for decreasing energies, starting from above this value, until $\mathscr{E}_T \approx 0.06$. Below this lower threshold, non-vanishing magnetization values reappear, indicating the existence of another transition. The magnetization fluctuation plots corresponding to this new transition are shown in figure 5 for lattice sizes up to 512×512. Note that fluctuations are drastically reduced below the maxima for each size. Note also that this transition occurs in the same energy range as the periodic-chaotic one observed in the pure Q2R [12] ($\mathscr{E}_p \approx 0.063$ was measured for 64×64 lattices).

In order to estimate both the critical energy value and the critical exponents for this new transition, we used the same data presented in figure 5 for energies above the maxima to construct the data collapsing plots of $\Delta^2 m L^y$ against $(\mathscr{E} - \mathscr{E}_T) L^x$. The parameters $\mathscr{E}_T = 0.0485$, $x = -0.95$ and $y = 1.83$ are chosen in order to optimize the

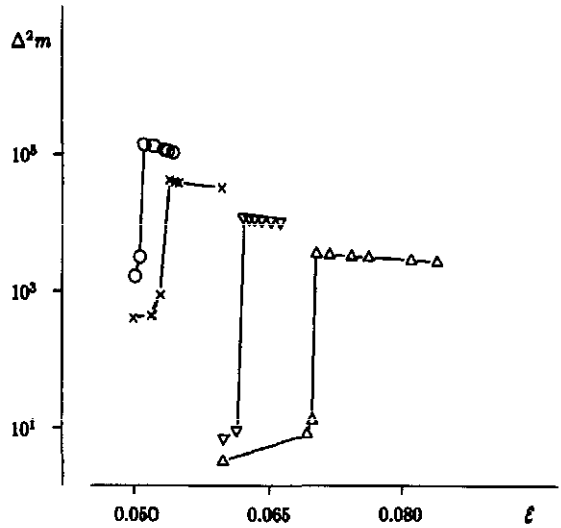

Figure 5. Mean squared fluctuation of the magnetization as a function of the energy, obtained from our second modified CA rule. The vertical scale is logarithmic. Circles represent data obtained from 512×512 lattices, crosses correspond to 256×256, inverted triangles to 128×128 and upright triangles to 64×64. The lines are guides to the eye.

collapsing. As the Onsager universality class corresponds to $x=-1$ and $y=1.75$, one is inclined to suppose that this transition may belong to this class. Instead of the optimized exponents, figure 6 was constructed by using the Ising values $x=-1$ and $y=1.75$, in order to test this hypothesis. Note that only the data corresponding to the smallest sizes 64×64 and 128×128 present small deviations far from the critical point (the scale is now linear). Using the optimized values one obtains a better collapse. Other data collapsing plots below each maximum for both the fluctuations and the

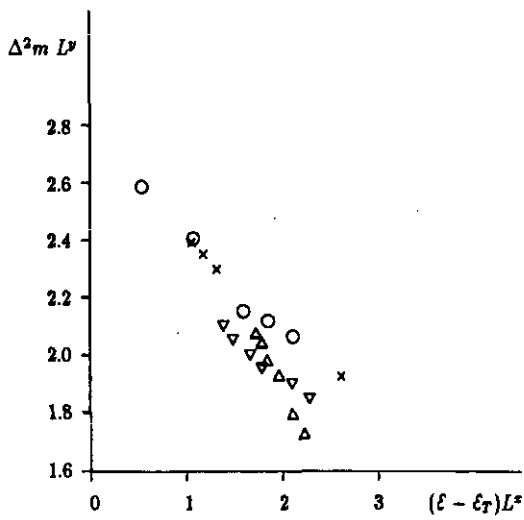

Figure 6. Data collapsing plot constructed using the same values of figure 5, above the maxima. The lattice sizes are represented by the same symbols as in figure 5.

magnetization are compatible with the same results, i.e. $\mathscr{E}_T = 0.049$ and Onsager exponents.

A possible interpretation for these results is that the additional flipping of two spins with local energies 0 and 4 is enough to allow the system to jump from one half phase space (with positive magnetization, for instance) to the other, resulting in a zero magnetization. However, this mixing of states is only possible when the system is above the periodic-chaotic threshold $\mathscr{E}_p$. Below this energy value, due to the formation of compact islands of spins with the same period [12], the additional flip of only one spin would be not enough to destroy the collective dynamic behaviour of such a whole island, giving rise to the reappearance of the Ising order. In other words, when the system is in the periodic phase, the spins are unable to jump from one half phase space to the other, in the thermodynamic limit. According to this interpretation, the various symmetries of the ordered Ising phase are maintained and the critical exponents remain the same, in agreement with the experimental results. The drastic lowering of the fluctuations below $\mathscr{E}_T$ seems to confirm this interpretation.

For this second modified rule, the average number of complete lattice updates is $\sim 10^7$. We noted a systematic curious feature. During the time evolution, the average fluctuations first seem to stabilize at some value, remaining nearly constant for many updates. Then they increase rapidly to another definitive value. The beginnings of these two plateaux differ from sample to sample, but the final value is nearly the same for all of them, even for samples where both plateaux are already completed after 10^3 steps, we observed no additional values until 10^7 steps.

4. Conclusions

The use of the Q2R cellular automaton as a microcanonical simulator for the Ising model is discussed. In particular, the distinct non-ergodicity degree presented by this automaton when compared with the true Ising dynamics below the critical point leads to underestimated measures of the fluctuations. We defined two modifications in the traditional Q2R dynamic rule, measuring the magnetization and its fluctuations for the square lattice. In the first modified rule, by enhancing the mobility of the energy quanta stored in broken bonds, we succeeded in reproducing the expected results. In this case, however, the local character of the energy transport was maintained, i.e. only small-length-scale movements are allowed, as in the Q2R traditional rule.

In our second modified rule, we included a much smaller change in the Q2R dynamics, as compared with our first modification, but now allowing large-length-scale energy transport. The Ising transition disappears, and another unknown transition was detected far below the Onsager critical point. The critical exponents corresponding to this new transition were measured, and their values coincide with the Onsager ones. The critical point, on the other hand, coincides with the energy for which a second transition was observed in the Q2R traditional dynamics [12]—below this value the system presents clusters of neighbouring spins oscillating with the same finite period, whereas above this value no periodic behaviour was found (the mean size of these clusters seems to 'blow up' at the critical point, as in the percolation problem [12]). A possible explanation for the relation of these three transitions is proposed.

The simulations were carried out on a 80286-based personal computer, running at 12 MHz.

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