COMMENT

Spin dynamics confinement in Q2R

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Abstract. For low concentrations, the occupied sites in Q2R cellular automata on the square lattice are known to be confined to the smallest rectangles surrounding them. However, they do not necessarily fill out the whole rectangle allowed for them. The effective confinement transition is found numerically to agree well with that of bootstrap percolation.

In Q2R cellular automata [1] on the square lattice, the sites initially are occupied with probability p and empty with probability $1 - p$. In the following dynamics, a site flips its status if it has as many occupied as empty neighbours. This approximation of the spin-$\frac{1}{2}$ Ising model mimics a microcanonical ensemble with constant energy but is not ergodic [2]. Nevertheless it seems to give correct Ising results provided one waits long enough or starts with an Ising configuration [3, 4].

In Q2R dynamics on the square lattice, a group of occupied sites in an otherwise empty lattice will always be restricted to the smallest rectangle surrounding it; all the empty sites surrounding that rectangle have three or four empty neighbours and thus never become occupied [1]. However, the corners of such an occupied rectangle do not necessarily remain occupied in the dynamical evolution, and it is not clear if in the later development all sites of an initially only partly filled rectangle will become occupied. If in a large and mostly empty lattice there are several groups of occupied sites, and if the surrounding smallest rectangles do not overlap, the occupied sites remain restricted to their rectangles; if the rectangles overlap or touch, the largest common rectangle surrounding the joint set of points defines the borderline of spin confinement. If this largest rectangle spans the lattice, the occupied sites might later be found nearly everywhere; if we have only finite distinct rectangles, each group of occupied sites remains confined to its own rectangle during all later iterations, and no information is spread. Rectangles are distinct in the Q2R dynamics if they are separated by a double line of empty sites.

The question under what conditions the surrounding rectangles join into a percolating network is known from bootstrap percolation [5, 6] and has been used there [7] as a cluster-flipping algorithm in the spirit of Swendsen–Wang dynamics of Ising models. In bootstrap percolation on the square lattice, an empty site becomes occupied if at least two of its four neighbours are occupied; occupied sites stay so forever. (Usually in bootstrap percolation the role of empty and occupied is reversed; the present notation corresponds to aspects of diffusion percolation [5].) Here the rectangles do fill up completely, if initially they were only partly occupied. Again, occupied rectangles stay distinct if separated by empty double lines. In $L \times L$ lattices, the surrounding rectangles merge into one network finally occupying the whole lattice if the initial concentration p is above the size-dependent [6, 8] threshold $p_c = 0.24_5/\ln(L)$.

Thus we want to know if in Q2R the rectangles surrounding the initially occupied sites also finally fill up and make that problem equivalent to bootstrap percolation.

A simple test shows that this is not the case. If we mark all sites which have been occupied at least once during the Q2R evolution, the resulting clusters are often but not always rectangular; figure 1 shows one of the exceptions. Thus there is no exact correspondence of Q2R and bootstrap percolation. Instead, we now ask if at least the thresholds p_c of Q2R and bootstrap percolation agree: critical points can be the same even if minor differences exist between different models.

What Q2R threshold should we take? The Curie point at 8% concentration is roughly independent of size and clearly unrelated to bootstrap percolation. The cluster period threshold [9] of Q2R is numerically difficult to determine accurately, and the damage-spreading threshold [4] for Q2R depends on both the observation time and the initial damage (single site versus whole line). Thus we select a threshold definition closer to the above ideas of spin confinement: for p below this threshold, the set of sites marked as occupied at least once during the development remains small and stays constant after some time; for larger p the concentration of sites marked in this way grows appreciably and reaches no plateau. To make a quantitative distinction, we made simulations up to a predetermined number t of sweeps through the lattice and called the spins in that sample confined if during the last 10% of the iterations no new sites became marked as occupied.
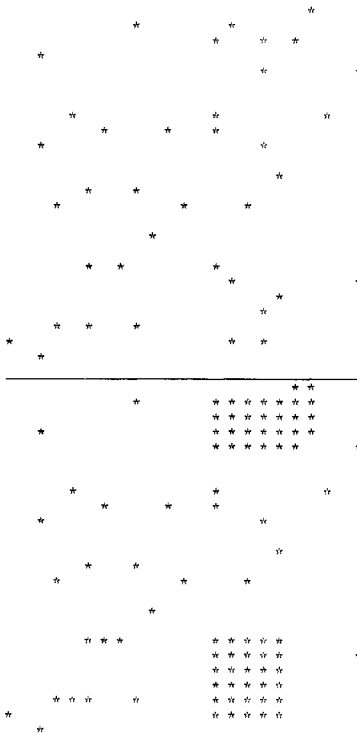

Figure 1. Example of a 23 × 24 Q2R lattice. The upper part shows the initially occupied sites, the lower part the sites marked as at least once occupied ($p = 0.065$). After 19 sweeps no additional sites were marked in this simulation; the total period of the limit cycle was 6230 sweeps on this example.

We used the Herrmann-type [4] vectorised multispin algorithm with 10^9 updates per second and per Cray processor. For each system size L we varied the initial concentration p until 5 out of 10 samples had confined spins. No systematic variation with observation time t from 10^3 to 10^5 iterations was found except for the largest lattices at short times. The effective threshold concentrations were 0.054, 0.043, 0.039 and 0.032 for $L = 128$, 384, 1152 and 3968, with errors of about 0.002. (For $t = 1000$ we found 0.026 and 0.021 for $L = 3968$ and 12 032; for $t = 100$ already at $L = 128$ a threshold of only 0.044 was observed; apparently observation times t smaller than the system size give systematic errors.) These data are in reasonable agreement with the above result $0.245/\ln(L)$ for bootstrap percolation [6]. (The prefactor is smaller if we demand that no new sites become occupied from time $t/2$ to time t.) Thus the logarithmic time dependence of some damage-spreading thresholds is replaced by a logarithmic size dependence for the confinement threshold and makes confinement similar to bootstrap percolation.

In addition we measured the median times to reach a plateau in the number of sites marked as occupied at least once. For that purpose, the concentration p was fixed at 0.044 within the region of the above thresholds. We checked how many iterations were needed until, during the latter half, the set of marked sites no longer increased. These times fluctuated by several orders of magnitude. Their medians were 130, 1730, 2200, 180 000 and 5×10^6 for $L = 128$, 256, 384, 512 and 640, from 100 runs each (except from 10 runs at $L = 640$). Figure 2 shows these data as well as the corresponding results up to $L = 1152$ if only during the last tenth of the simulation, the number of marked sites was required to be constant. An exponential size dependence of this confinement time is clearly visible, with periods reminiscent of Q2R limit cycles [2], but easier to measure since now the times for the same L are much shorter. This result at first seems at variance with the above observation that the effective threshold is independent of time for large times. However, the exponential dependence of time on length means a logarithmic dependence of length on time, and thus a
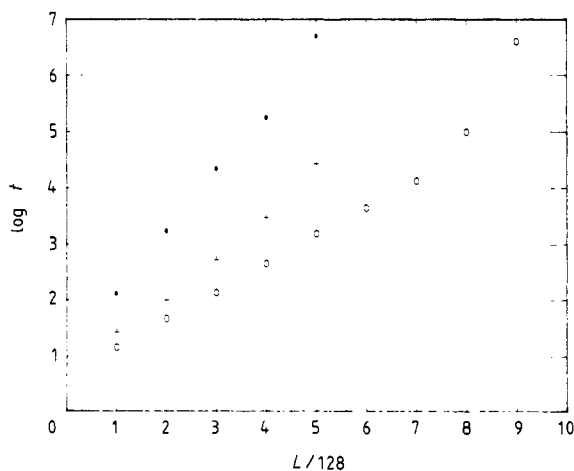

Figure 2. Semilogarithmic plot of median time (decadic logarithm) at $p = 0.044$ against linear system dimension L (in units of 128). The data refer to a plateau during the latter half (upper data, ●) or latter 10% (lower data, ○) of the observation time. The + data in the middle show for comparison the median total period of the limit cycle at the much lower concentration 0.012, similar to [2].

log(log t) dependence of the threshold on time. This log–log dependence of the effective thresholds on observation time, that results from the exponential behaviour in figure 2, is probably too weak to be detected from our numerical data.

We thus found a logarithmic size dependence of the confinement transition in Q2R; the small influence of the observation time is explained through the exponential size dependence of the times involved. The work took 39 h execution time on a Cray-YMP processor.

References

[1] Vichniac G Y 1984 *Physica* **10D** 96
    Pomeau Y 1984 *J. Phys. A: Math. Gen.* **17** L415
    Herrmann H J 1986 *J. Stat. Phys.* **45** 145
[2] Schulte M, Stiefelhagen W and Demme E S 1987 *J. Phys. A: Math. Gen.* **20** L1023
[3] Moukarzel C 1989 *J. Phys. A: Math. Gen.* **22** 4487
[4] Glotzer S C, Stauffer D and Sastry S 1990 *Physica* **164A** 1
    Herrmann H J 1986 *J. Stat. Phys.* **45** 145
[5] Adler J and Aharony A 1988 *J. Phys. A: Math. Gen.* **21** 1387
    Manna S S, Stauffer D and Heermann D W 1990 *Physica* **162A** 20
[6] Nakanishi H and Takano H 1986 *Phys. Lett.* **115A** 187
    Adler J, Stauffer D and Aharony A 1989 *J. Phys. A: Math. Gen.* **22** L297
[7] Adler J, Gross R and Warmund R 1990 *Physica* **163A** 440
    Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86
[8] Aizenman M and Lebowitz J L 1988 *J. Phys. A: Math. Gen.* **21** 3801
    Schonman R H 1990 *J. Stat. Phys.* **58** in press
[9] Herrmann H J, Carmesin H O and Stauffer D 1987 *J. Phys. A: Math. Gen.* **20** 4939