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1994 J. Phys. A: Math. Gen. 27 6955

(http://iopscience.iop.org/0305-4470/27/21/012)

J. Phys. A: Math. Gen. 27 (1994) 6955–6962. Printed in the UK

Critical behaviour of non-equilibrium q-state systems

Andrea Crisanti† and Peter Grassberger‡

† Dipartimento di Fisica, Università di Roma I, Ple. Aldo Moro, Roma, Italy

‡ Physics Department, University of Wuppertal, D-42097 Wuppertal, Germany

Received 28 July 1994, in final form 13 September 1994

Abstract. We present two classes of non-equilibrium models with critical behaviour. Each model is characterized by an integer $q > 1$, and is defined on configurations of q-valued spins on regular lattices. The definitions of the models are very similar to the updating rules in Wolff's algorithm for the Potts model, but both classes break detailed balance, except for $q = 2$ and $q = \infty$. In the first case both models reduce to the Ising model, while one of them reduces to percolation (more precisely, to the general epidemic process) for $q = \infty$. Locations of the critical point and critical exponents are estimated in two dimensions.

It is by now well understood that non-equilibrium models can show critical behaviour very similar to second-order phase transitions in equilibrium systems. Indeed, dropping the requirement of detailed balance gives additional freedom, and one can observe a much richer spectrum of possibilities. These include, in particular, critical behaviour for generic values of the control parameters, i.e. systems which do not require the control parameter to be set to any non-natural value to be critical. Examples for this are diffusion-limited aggregation [1, 2] and various models of self-organized criticality [3–5].

A problem which is more common in non-equilibrium models than in equilibrium cases is that it is often not clear how large the universality classes are. Thus, for example, it is not yet clear whether different versions of the sand-pile model [3, 6] are in the same universality class or not. Another much discussed example is provided by models with an absorbing state. The prototype of such models is directed percolation, interpreted as an epidemic process without immunization. By now it seems clear that a model for heterogeneous catalysis proposed some years ago by Ziff *et al* [7] does belong to the same universality class, in spite of original numerical indications to the contrary [8]. But there still exist a number of similar models (some with degenerate absorbing states) for which conflicting evidence has been reported concerning universality.

Another problem which is more frequent in non-equilibrium cases is that no good field-theoretic treatment exists. The best known example for this is diffusion-limited aggregation which is still not amenable to such a treatment. This does not mean that one cannot write down 'Hamiltonians' [9, 10] or path integrals [11], but rather that no good perturbation expansions are available which could then be resummed by renormalization-group methods. Other models for which this applies are the sand-pile model [12] and 'true' self-avoiding walks [13, 14] for which the field theories are intrinsically non-renormalizable [15].

In the present paper we want to present two new classes of non-equilibrium critical phenomena. They are superficially similar to the Potts model [16], but they are not defined in terms of Hamiltonians. Instead, they are defined algorithmically, by stating the rules for

0305-4470/94/216955+08$19.50

updating the state of a system. This is similar, for example, to the sand-pile model. But in contrast to that, our models show 'conventional' critical behaviour in the sense that they involve control parameters, the critical behaviour only being observed for special values. On the other hand, we have not yet been able to apply field-theoretic methods to them.

Both class of models involve 'spins' with q possible orientations ('colours'), and are symmetric under cyclic permutations of the colours. In addition, the first model is invariant under the exchange of any two colours, just as the Potts model is. The rules for updating a configuration are very similar to Wolff's single-cluster variant [17] of the Swendsen–Wang dynamics [18] of the Potts model. Thus let us recall Wolff's algorithm as applied to the q-state Potts model.

Assume we have a configuration of spins on a hypercubic d-dimensional lattice, with spin values s_i, $i \in Z^d$. The evolution is defined by sequential updatings of randomly selected clusters. To make one update, we proceed as follows.

(i) We pick a random colour $s \in [0, 1, \ldots q-1]$.
(ii) Pick a random site $i \in Z^d$. If $s_i = s$, we do not do anything and proceed to the next update.
(iii) Otherwise, we build a *bond* percolation cluster on the subset of sites j which have $s_j = s_i$ and which are connected to i.
(iv) After this is done, we flip this cluster, i.e. we change all its s_j to s, and proceed to the next update.

The control parameter in this model is the probability p for connecting sites in the percolation process in step (iii). It is related to the interaction strength K in the Potts model, $e^{-\beta H} = \exp(K \sum_{\langle i,j \rangle}(\delta_{s_i,s_j} - 1))$, by $p = 1 - e^{-K}$ [18].

Our first class of models ('class A') is obtained from this algorithm by keeping steps (i), (ii) and (iv), but replacing step (iii) by

(iiiA) Build a bond percolation cluster on the sites j which are connected with site i and which have $s_j \neq s$.

Again this is done with probability p for each bond. But for this model we were not able to prove detailed balance for general values of q, and we thus cannot relate p with a coupling strength in any Hamiltonian.

In the second class of models ('class B') we skip step (i), keep step (iii), and replace the other steps by

(iiB) Pick a random site $i \in Z^d$.
(ivB) Flip all spins of the percolation cluster into colour $s_i + 1 \bmod q$, i.e. rotate the entire cluster in colour space by an angle $2\pi/q$.

In this model the braking of detailed balance is evident.

The simplest case is $q = 2$. In this case, the Potts model goes over into the Ising model if we perform the trivial relabelling $s = 0 \rightarrow s = -1$. It is easy to see that, in this case, models A and B are also equivalent to the Ising model.

Another simple limit is $q = \infty$. In this limit, s_j will be different from s with probability 1, and thus the cluster built in step (iiiA) is just an ordinary bond percolation cluster on the entire lattice. Thus model A is equivalent to the spreading of bond percolation according to the general epidemic process [19] or the Leath algorithm [20].

The $q \rightarrow \infty$ limit of model B is rather different. It is easy to see that there is no ordering for any finite p in this limit. For finite q and p, there is a balance between ordering due to the fact that two sites i, k which originally had $s_j = s_k - 1$ might get the same colours by flipping j, and disordering because a coherent cluster is broken up. For $q \rightarrow \infty$, the

ordering disappears, and thus the transition point has to shift to $p_c \to 1$. For $q = \infty$ all clusters are trivial (just one site) for all p, suggesting that the transition turns into first order (all scaling law amplitudes $\to 0$) for $q \to \infty$. Notice that this conclusion rests on the fact that the fractal dimension of percolation clusters at $p \leqslant p_c$ is zero, whence the ordering by each cluster flip effects only a vanishing fraction of sites, and a random initial configuration remains essentially random. This is not so on finite lattices (in particular at $d = 2$), since there the co-dimension of percolation clusters is very small, and hence typical cluster flips involve large parts of lattice. Thus we expect very large finite-size effects in model B even for finite values of q.

Next let us discuss mean-field theory. In both models, this implies that a spin not yet checked during the build-up of a cluster has the same probability $1/q$ to have any of the q possible colours. In a strict mean-field treatment one would also assume the same for sites which had already been visited during the present cluster evolution. In the following we shall discuss a more realistic 'hybrid' mean-field ansatz where we do not make the latter approximation. In this case both models reduce to mixed-site bond percolation. In model A we have bonds established with probability p, and sites with probability $1 - 1/q$. In model B, the bond probability is the same, but the site probability is $1/q$. This implies correctly that model A turns into bond percolation for $q \to \infty$. But it predicts a qualitatively wrong behaviour for model B, as it would imply that model B does not become critical for $q > 1/p_{c,\mathrm{site}}$, where $p_{c,\mathrm{site}}$ is the threshold for site percolation on the same lattice. This is obviously a weakness of our mean-field ansatz, as it would mean that even the Ising model ($q = 2$) is non-critical in two dimensions. The same problem would occur for the strict mean-field treatment mentioned above, and for the original Swensen–Wang–Wolff model with $q > 2$.

In the following we shall report results from simulations on 2D square lattices of size $N \times N$ with periodic boundary conditions. We used both depth-first [21, 22] and width-first ('Leath' [20]) algorithms for building the percolation clusters. While the first are somewhat simpler when implemented by recursive function calls, the temporal behaviour is more natural in the latter as it corresponds to epidemic-like spreading [19]. The critical point and the distribution of cluster sizes (and of cluster radii) is identical with both algorithms. In all cases a sufficient number of cluster flips during the initial transient stage was discarded, i.e. all data reported below refer to the stationary state.

In order to obtain p_c for model class A, we used two different procedures. In the first (finite-size scaling) we used relatively small lattices (up to $N = 1024$), and determined $p_{c,N}$ from the requirement that the cluster size distribution $P_N(s)$ shows the longest scaling region for this value of p. In figure 1 this is illustrated for $q = 3$ and $N = 1024$. Values of $p_{c,N}$ resulting from this and analogous plots are plotted against $1/N$ in figure 2. We see a straight line for $N \geqslant 200$ which extrapolates to

$$p_c = 0.5330 \pm 0.0004 . \tag{1}$$

In the second procedure, we used much larger lattices (up to 8192×8192) and sufficiently small values of p so that all cluster diameters were $\ll N$ and finite-size effects were negligible. In figure 3, resulting average cluster sizes $\langle s \rangle$ are plotted against $p_0 - p$ for three different values of p_0. Since we expect

$$\langle s \rangle \sim (p_c - p)^{-\gamma} \tag{2}$$

we expect a straight line at $p_0 = p_c$. This is indeed observed, with the same p_c as above and with $\gamma = 1.65 \pm 0.05$. The error is mainly systematic due to a slight but significant curvature in figure 3.

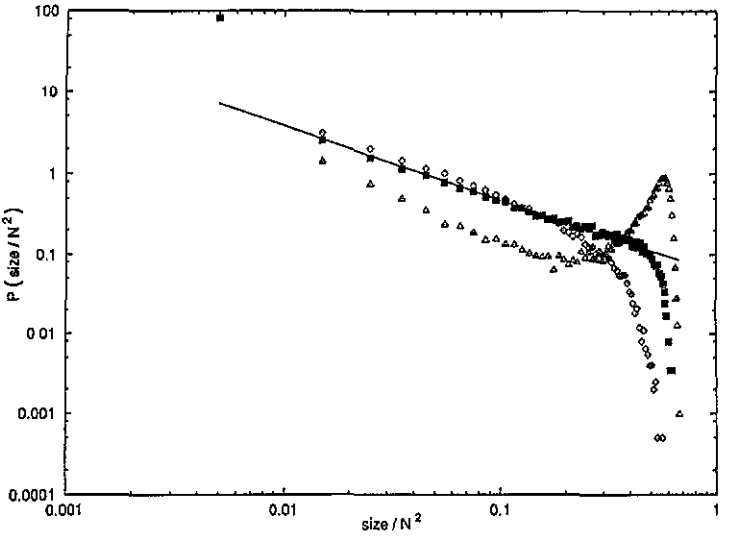

Figure 1. Cluster-size distributions for $q = 3$, lattice size $N = 1024$ and three different values of p: $p = 0.531\,75$ (◇), $p = 0.532$ (■), and $p = 0.532\,25$ (△). Data were binned into bins of size $\Delta s = 10^4$. The straight line has slope -0.9.

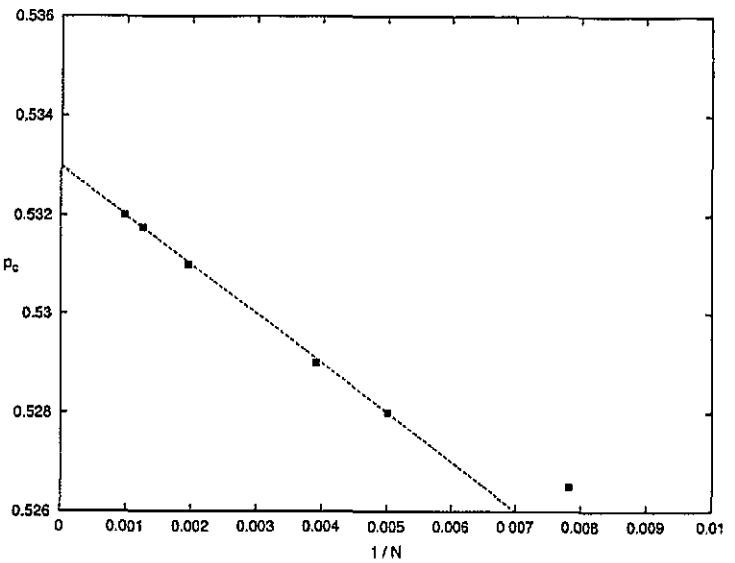

Figure 2. Finite-size critical values $p_{c,N}$ versus $1/N$ for $q = 3$. For large N the data seem to follow a straight line, the extrapolation of which to $1/N = 0$ gives p_c (broken line).

Similar deviations form scaling behaviour are seen in the average cluster evolution times and in the size distribution $P(s)$. The former satisfies

$$\langle T \rangle \sim (p_c - p)^{-\delta} \qquad \delta \approx 0.85 \tag{3}$$

(see figure 4), but there are rather strong deviations from a pure scaling law.

From figure 1 we see that the distributions $P_N(s)$ on finite lattices at $p = p_{c,N}$ fulfill

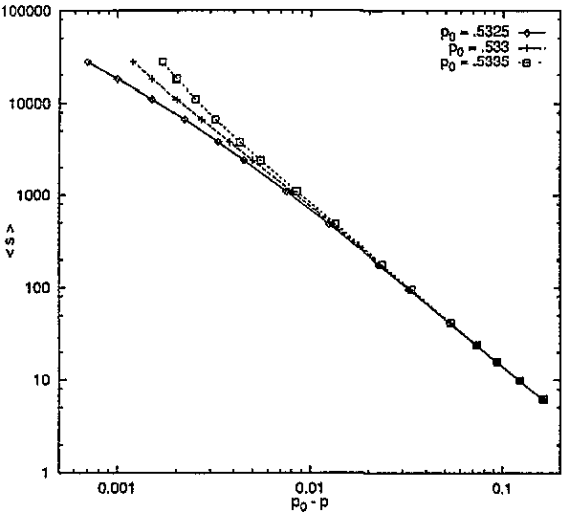

Figure 3. Log–log plot of average cluster size for $q = 3$ against $p - p_0$, for $p_0 = 0.5325, 0.533$ and 0.5335. A roughly straight line is seen for $p_0 = p_c \approx 0.533$, but notice that there are small but significant deviations.

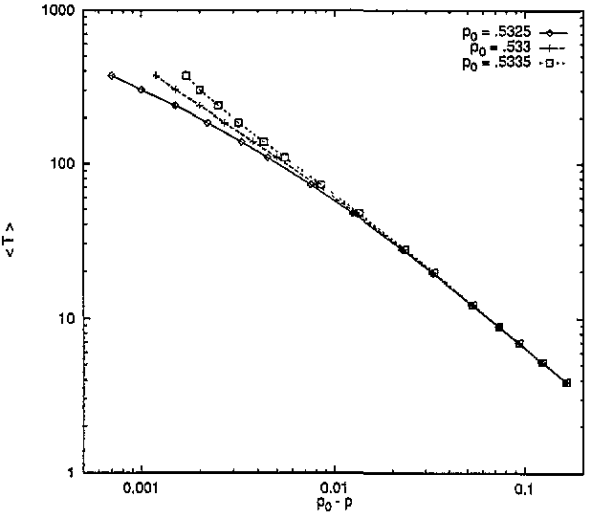

Figure 4. Same as figure 3, but for the average cluster lifetime.

roughly a scaling law

$$P_N(s) \sim 1/s \tag{4}$$

for $s \ll N^2$, i.e. in the usual notation [23] we have $\tau \approx 2$. Results for larger lattices and $p < p_c$ are shown in figure 5. We see there again roughly $P(s) \sim 1/s$ for $s < (p_c - p)^{-\gamma}$ (notice that bin sizes are $\propto s$ in figure 5, in contrast to fixed bin sizes in figure 1). But this is superimposed by oscillations whose amplitude increases as we approach the critical point. The latter is very different from the Ising ($q = 2$) and percolation ($q = \infty$) limits, but was also observed for $q = 4$ and for the time distribution for $q = 3$ and $q = 4$. On the other

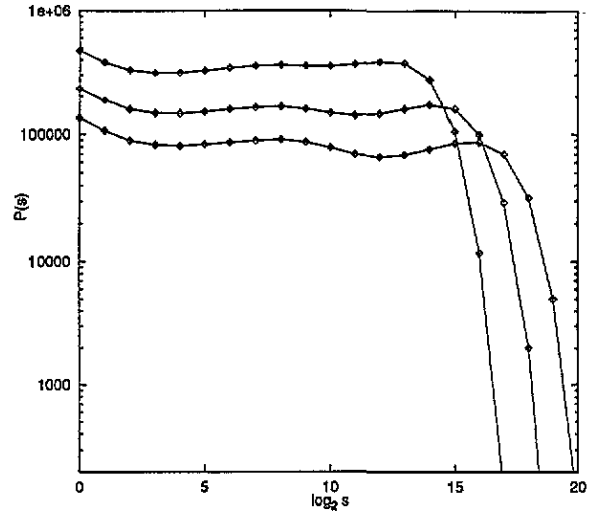

Figure 5. Cluster size distributions ($q = 3$) for subcritical p on practically infinite lattices. Values of p are 0.5292, 0.531, and 0.5318. Data are binned into bins $[s, 2s-1]$.

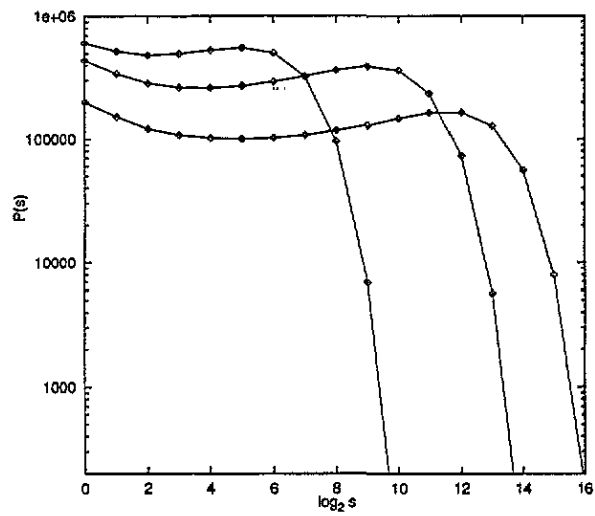

Figure 6. Similar as figure 5, but for model B with $q = 3$. Values of p are 0.61, 0.63, and 0.6326.

hand, model B leads to cluster-size distributions which are qualitatively as in percolation and in the Ising model, see figure 6.

Results for p_c and for the critical exponent γ are summarized in table 1, for both model classes. For class A, we see that p_c interpolates monotonically between the Ising and percolation limits. The latter is approached very quickly. On the other hand, γ seems first to fall below the Ising value $\frac{7}{4}$, and rises only very slowly towards the percolation limit $\frac{43}{18} = 2.388$ for $q \to \infty$. For class B we see that there is a phase transition for all values of q with $p_c(q) \to 1$ very slowly for $q \to \infty$. The amplitudes in the scaling laws for class B seem to tend towards zero for $q \to \infty$ (the clusters become very small except when p is very near p_c), in agreement with the arguments given above. We do not quote exponents

Table 1.

	$q=2$	$q=3$	$q=4$	$q=8$	$q=\infty$
Model A:					
p_c	0.5858	0.5330	0.5170	0.5029	0.5
γ	1.75	1.65	1.79	1.88	2.388
τ	2	≈ 2	≈ 2	≈ 2	2.055
Model B:					
p_c	0.5858	0.633	0.6667	0.7393	1
γ	1.75	1.35	1.21	0.71	—

δ because they are very strongly affected by corrections to scaling, and we do not quote exponents τ for class B for the same reason.

Superficially, our models resemble the Potts model. There, one has a first-order transition for $q > 4$. Thus one might wonder whether there is some range in q in which one of our models also has a first-order transition. We have not found any indication for that.

In summary, in this paper we have presented evidence for two new classes of non-equilibrium critical phenomena. Both classes use Potts spins, and are defined via cluster evolution rules similar to those of the Wolff dynamics for the Potts model. The most interesting aspect of the first class is that it interpolates between the Ising model ($q = 2$) and percolation ($q = \infty$). For this class we have not been able to find any observable which shows broken detailed balance. We thus cannot exclude that an equilibrium version also exists for this model, possibly with long-range interactions (otherwise it would be hard to understand why these models have not been found before).

In class B, breaking of detailed balance is evident. Indeed, the transition in class B is from desynchronized cyclic behaviour to synchronized by formation of a percolating cluster of sites with common phase. Synchronization in spatially extended models was studied recently in [24, 25]. In [24] it was argued that no synchronization can occur in stochastic discrete models with > 2 states. Continuous models were studied in [25] where a connection was established with surface roughening in Kardar–Parisi–Zhang growth. The latter suggests that no phase transition with long-range order occurs in $d = 2$ for such models either. These predictions are in clear contrast to our findings. This reflects basic differences in the dynamics underlying model B and the systems studied in [24, 25]. While it is assumed in the latter that the phase proceeds rather uniformly with locally independent fluctuations, the phase progress in the ordered phase of model B is dominated by rigid flippings of entire large clusters.

Finally, we have neither done any simulations in $d > 2$, nor have we attempted a field-theoretic treatment. Using methods of [9–11] it should not be difficult to set up the field theory. But it might be much harder to find a systematic perturbation expansion.

Acknowledgments

Part of this work was done when one of us (PG) was visiting Rome University. He wants to thank A Vulpiani and G Paladin for their generous hospitality and for numerous enlightening discussions.

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