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2000 J. Phys. A: Math. Gen. 33 L465

(http://iopscience.iop.org/0305-4470/33/48/101)

J. Phys. A: Math. Gen. **33** (2000) L465–L470. Printed in the UK PII: S0305-4470(00)17071-4

LETTER TO THE EDITOR

Branched polymers and percolation

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Received 11 September 2000

Abstract. We study a supposed model for branched polymers which was shown in two dimensions to be in the universality class of ordinary percolation. We confirm this by high-statistics simulations and show that it is in the percolation universality class also for three dimensions, in contrast to previous claims. These previous studies seem to have been misled by huge corrections to scaling in this model.

Although most statistical physicists have an intuitive notion of the concept of universality at second-order phase transitions, a rigorous method to delineate universality classes does not yet exist. As a consequence, again and again the problem arises of whether two specific models are in the same universality class or not. If critical exponents can be obtained exactly, then one can at least say when they are not in the same class: if the exponents do not coincide, but in general one has to resort to numerical methods, such as series expansions or Monte Carlo simulations. Since both require extrapolations in order to obtain critical exponents, it is not surprising that wrong claims about universality classes appear again and again.

Several years ago, a model was introduced in [1] (called LATST in the following) which was supposed to describe the growth of branched polymers in a disordered medium. Branched polymers in thermal configurational equilibrium are in the universality class of lattice animals [2]. This is an ensemble of connected clusters of sites on a regular lattice where all configurations with the same number of sites have the same weight.

The LATST model is different. It is defined kinetically. It lives on a randomly diluted hypercubic lattice, such that monomers can be placed only on a fraction p of lattice sites. Starting with a monomer as an active point seed, at each time step the oldest active site is chosen and its free neighbours (usable but not yet used) are counted. If there is no free neighbour, the site becomes inactive and the next active site in the list is chosen. Otherwise, one of the free neighbours (chosen randomly) is declared a new active site. In addition, if there is another free neighbour, a second site is made active with probability b. This is called 'branching'. After this is done, the old active site is also made inactive and the next active site is chosen from the list. When p is smaller than a critical value p_c, then the process dies with unit probability for all values of b. For $p > p_c$, there exist a critical value $b_c = b_c(p_c)$ such that it has a non-zero chance to survive for $b > b_c(p_c)$.

Obviously this is very similar to the growth of an epidemic in the general epidemic process ('dynamical percolation') [3]. In the latter, the main difference is that all neighbours of an active site have the same chance p of being activated, independent of how many others can be or are activated. Thus, if a site has m neighbours not yet occupied, the number of its

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'descendants' is a Poissonian random number with average $p\,m$. In contrast, in the LATST model the variance of the number of activated descendants is reduced. It is always either zero, one or two, and never greater than two. This difference is most pronounced for $p = 1$ and for lattices with high coordination number, because then b_c is very small (see below) and most of the time there is just a single descendant. However, we should not expect this to be relevant in the renormalization group sense, i.e. we should expect that the LATST model is in the universality class of the general epidemic process and hence of ordinary percolation. In some sense, LATST and the general epidemic process are related to each other like the 'growing self-avoiding walk' (GSAW) [6, 7] and the usual self-avoiding walk (SAW), which are also known to be in one common universality class.

The transition in the two-dimensional LATST model was indeed found to be in the percolation universality class in [4]. For $d = 3$, the same was verified in [4] for values of p close to p_c, but not for $p = 1$. In [5] it was claimed that the latter shows clean scaling which is definitely not in the percolation universality class. We claim here that this is wrong. With present-day computers it is practically impossible to obtain the scaling regime for the case $d = 3$, $p = 1$, but all numerical evidence hints at the fact that the model is in the percolation universality class.

In order to see the origin of the problem, we notice that the LATST model is for $p = 1$ and $b = 0$ just the GSAW. As already pointed out, this is in the SAW universality class, but it has greatly reduced attrition since monomers are placed only on free neighbours in the GSAW, while they are placed at randomly chosen neighbours (whether they are free or not) in SAWs. As a consequence, the attrition constant (the rate with which the process dies) is 0.024 in $d = 2$ and 0.000 275 in $d = 3$. Thus, in order to overcome attrition, it would be sufficient to make an enrichment step [8] every 40 time steps in $d = 2$, and every 3600 time steps in $d = 3$. These give lower estimates $b_c(p = 1) \geqslant 0.024(d = 2)$ and $b_c(p = 1) \geqslant 0.000\,275(d = 3)$. Indeed, the actual estimates for b_c are rather close to these: $b_c(p = 1) = 0.056$ [4] for $d = 2$ and $b_c(p = 1) = 0.000\,34$ [5] for $d = 3$. Since $1/b$ sets a timescale (the average time between two branchings), this shows that there are large inherent times $T \approx 20$ and $T \approx 3000$ respectively in the LATST model. Any critical scaling is expected to show up only for $t \gg T$. While such t are still feasible in high-statistics simulations in two dimensions, they are out of reach in three dimensions.

To verify these predictions, we performed simulations. We studied only the most difficult and controversial case $p = 1$: for $p < 1$ it seems accepted that the LATST model is in the percolation class. In order to reach large clusters without finite-lattice effects we used hashing. This allowed us to use virtual lattices of sizes up to $100\,000^3$, so we could study clusters of up to 10^6 sites without any finite-lattice corrections. Such corrections were obviously important in the figures shown in [5], but it is hard to judge from these figures what parts of the distributions are unaffected by them.

We used the fast and reliable four-tap random number generator of [9]. Each curve in the following figures is based on a sample with at least 3×10^5 clusters. Although this statistics is higher than previous ones [1, 4, 5] by several orders of magnitude, the entire project needed only about 200 h CPU time on fast workstations.

Mass distributions of two-dimensional clusters for five values of b are shown in figure 1. Actually, in order to take into account the very small error bars, we plotted not $P(M)$ itself but $M^{\tau-2}P(M)$ where $P(M)$ is the probability that a cluster has mass $\geqslant M$, and $\tau = 96/91$. This is motivated by the fact that $P(M) \sim M^{2-\tau}$ for two-dimensional percolation. Thus we expect our data to be flat for $b = b_c$, except for corrections to scaling. This is indeed the case for $M > 10^4$ and $b_c = 0.056\,80 \pm 0.000\,04$. The average square size $\langle R^2 \rangle$ obtained from the same runs is shown in figure 2. Again the asymptotic behaviour $R^2 \sim M^{96/91}$ expected for

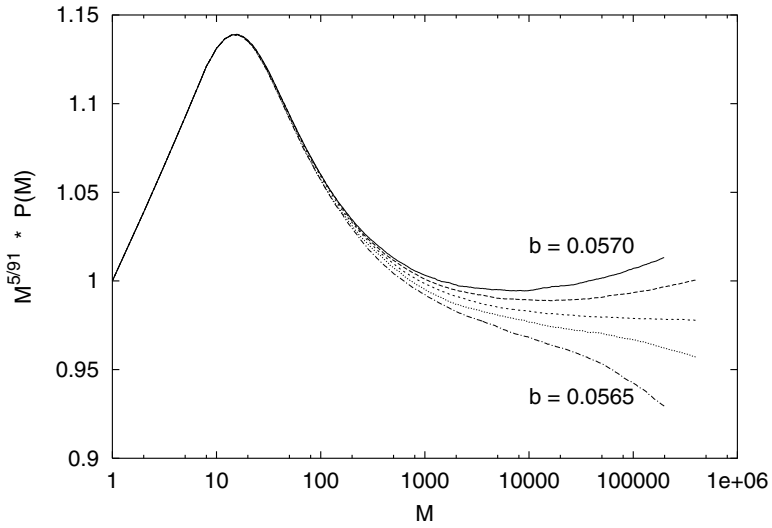

Figure 1. Log–linear plot of $M^{\tau-2}P(M)$ versus M for two-dimensional clusters. The curves are for $b = 0.057$, 0.0569, 0.0568, 0.0567 and 0.0565 (top to bottom).

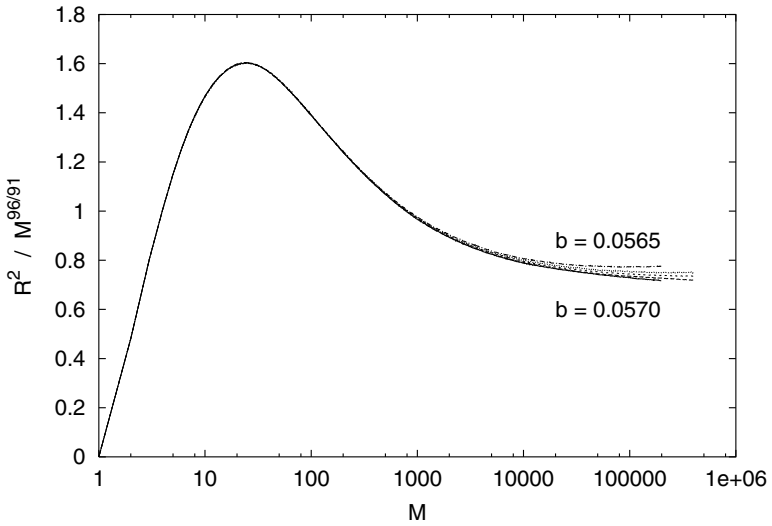

Figure 2. Log–linear plot of $R^2/M^{2/D_F}$ versus M for two-dimensional clusters, where $D_F = 91/48$ is the fractal dimension of two-dimensional percolation clusters. The curves correspond to the same b-values as in figure 1 (bottom to top).

percolation is divided out, and again we see flat curves for $M > 10^4$. Our estimate for b_c is in rough agreement with that in [4] but about ten times more precise (assuming that the error quoted on page 1744 of [4] is misprinted; otherwise it would be a factor of 100 more precise).

For $d = 3$, $M^{\tau-2}P(M)$ versus M is plotted in figure 3. For $\tau - 2$ we used the value 0.189 from [10]. We see clearly different behaviour for $M < 3000$ and for $M > 3000$. For $M < 1000$ we have the expected scaling of simple random walks. For $M \gg 3000$ we expect to see percolation, but this sets in only very late. Roughly straight lines in the range

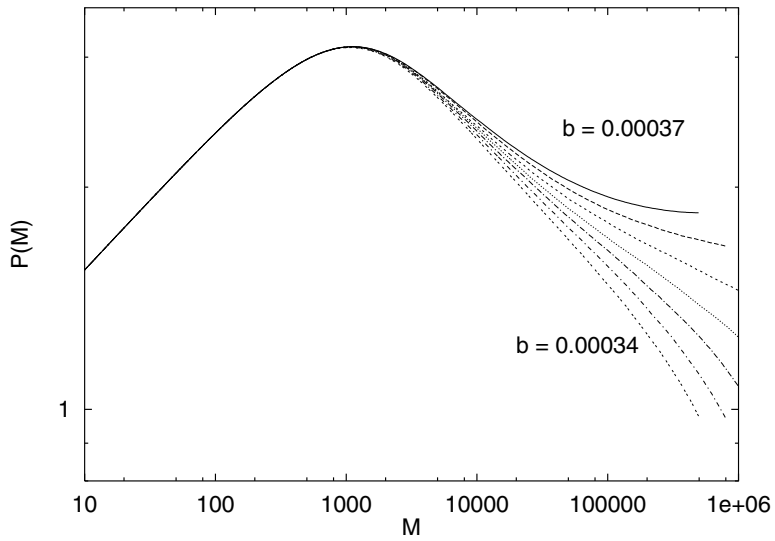

Figure 3. Plot of $M^{0.189}P(M)$ versus M for three-dimensinal clusters. The curves are for $b = 0.000\,37, 0.000\,365, 0.000\,36, \ldots, 0.000\,34$ (top to bottom).

$3000 < 10^5$ are seen for $b \approx 0.000\,34$. Obviously, the estimate $b_c = 0.000\,334$ of [5] was based on this range, although all log–log plots of [5] show straight lines in the entire range $M > 10^2$, for reasons which we do not understand. In any case, these straight lines do not represent the asymptotic behaviour, since all our curves except those for $b \geqslant 0.000\,36$ bend down for very large M (notice that each curve is based on independent runs, thus all systematic structures seen in any of our plots are significant). Indeed we estimate that the curve for $b = 0.000\,36$ in figure 3 will also bend down for $M > 10^6$, and the estimated critical value is $b_c = 0.000\,366 \pm 0.000\,004$.

Average values of the 'chemical radius' (the length of the paths connecting active sites to the seed) and of the number of active sites are shown in figures 4 and 5. Here we plotted the raw data themselves. We again see the break in scaling at $M \approx 3000$. A careful look at the data (e.g. plotting them again with some power split off) shows that the curves are not straight for $M \gg 3000$ but show similar curvature as $P(M)$. Thus also in these cases it is impossible to extract critical exponents from the data. In contrast to this, the authors of [5] found perfect scaling without visible corrections (and with exponents different from those for percolation) for all cluster masses $>10^2$ and chemical radii >10. We have no explanation for this.

In summary we have shown that it is extremely dangerous to estimate critical exponents from data which have important corrections to scaling. In the present case these corrections seem to have led to wrong claims about universality, but it is not clear why the authors of [5] have missed them. In any case we see no reason to doubt that the LATST model is in the universality class of percolation, for any finite dimension d. Numerical verification for $d \geqslant 4$ is of course out of the question.

Let us finally end with two comments. The first is that the subcritical process is not, as claimed in [1, 4, 5], in the universality class of SAWs. It is in the lattice animal universality class, like any model whose critical point is in the percolation class†. Secondly, it is not clear in

† This is at least true if one conditions on rare large clusters with fixed number of sites, as is usually done. If one conditions instead on clusters with large fixed chemical radius, then subcritical percolation (and thus also LATST) is in the SAW universality class.

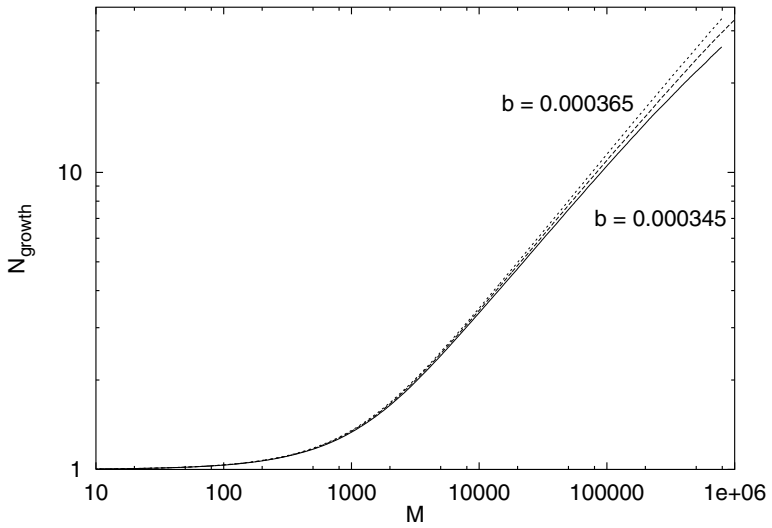

Figure 4. Number of active (growth) sites versus M for three-dimensional clusters. Only three curves are shown.

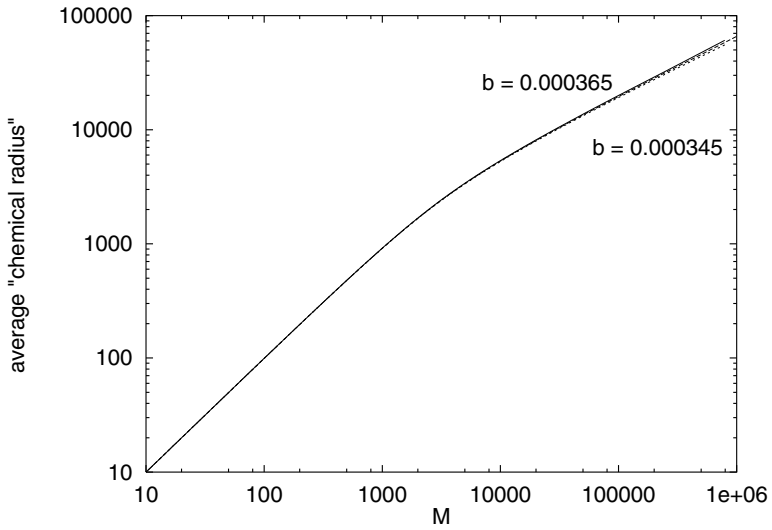

Figure 5. 'Chemical radius' (average shortest path length from seed to active sites) versus M for three-dimensional clusters. Only three curves are shown.

what sense the LATST model is a valid model for branched polymers (BPs). It certainly does not describe the ensemble of fully annealed BPs, except in the sense just mentioned (lattice animals are in the same universality class as BPs). It cannot describe either the ensemble of BPs in which branch points are frozen but bends between successive monomers are annealed (i.e. BPs with fixed topology), since this topology is determined in the LATST model by local configurations. It is for this reason that we have avoided the name 'branched polymer growth model' (BPGM) proposed in [4, 5].

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