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Growth model induced by a random walk of particles

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Abstract

In this paper, we present the numerical study of a model of the growth of geometrical structures. Particles are randomly placed on a two-dimensional (2D) square lattice and move as random walkers which annihilate when encountering an occupied site. The model is studied for two cases. In case A, we study the critical properties as a function of the initial particle concentration, C_I, after the annihilation of all particles. We have found a critical behaviour characterized by the emergence of a percolative cluster for $C_I^* = 0.098\,82 \pm 2 \times 10^{-4}$. In case B, we do a kinetic study of the systems where the fraction of occupied sites, q, is a measure of time. For C_I^* we obtain $q^* = 0.4679 \pm 0.0005$. This kinetic study is also done for $C_I = 0.2$, 0.3, 0.45 and 0.5927. The critical exponent ν and the exponent ratios $\frac{\beta}{\nu}$ and $\frac{\gamma}{\nu}$ are measured for all cases. We compare the results obtained with the known 2D percolation values. The results obtained suggest the existence, for an infinite system, of a critical line in the phase diagram $C_I - q$ (C_I is the particle concentration, q is the fraction of occupied sites), $q \sim (C_I)^{1-d'_f/2}$ (where $d'_f = 1.74$), connecting the points $(C_I^* = 0.098\,28, q^*(C_I^*) = 0.4679)$ and $(q^*_{perc}, q^*(q^*_{perc}))$ where $q^*_{perc} = 0.5927\ldots$ is the 2D square lattice critical site percolation parameter.

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1. Introduction

The modelling of the growth of structures has attracted the attention of many researchers. Growth phenomena can be found in a variety of situations, such as growth of tumours and bacterial colonies, colloidal aggregation, phase growth, gelation [1]. In spite of the complexity of these systems, it has been found that important aspects of their behaviour are captured by

phenomenological models. Some of these models are defined through stochastic rules and geometrical constraints play an important role.

In this paper, we study a model related to kinetic gelation models that has been intensively studied [2]. In the kinetic gelation models, monomers which occupy lattice sites are characterized by their functionality, i.e. the maximum number of bonds that they can form with their neighbours. Initially, there are no connections (bonds) between monomers. As time goes by, bonds are formed by the motion of an initiator agent and, after a critical time has elapsed, a macroscopic gel appears in the system. Bonds can only appear if an initiator agent moves from one monomer to another neighbouring monomer that still has a 'free' bond to form. Recently, reported studies have been consistent with kinetic gelation belonging to the percolation universality class [3].

The model we propose is related to kinetic gelation models in the sense that particle motion induces the growth of a percolating structure. A similar model has been considered as a model of crack growth in solids with many initial defects [4]. However, in this work, the authors considered a bond connectivity criteria, between clusters, as done in kinetic gelation, whereas we consider a site connectivity criteria. Our model can be seen as a model of the growth of disorder induced by the motion of many random walkers. The sites visited by the walkers become 'damaged' and behave as annihilation sites. Consequently, the walkers self-interact and interact with each other. These interaction and memory effects make the model non-trivial. The walkers we consider can also be seen to belong to the general class of active walkers [5] in the sense that they change the properties of the lattice where they are moving. Our consideration of site connectivity criteria means physically we consider that, when two neighbouring sites are 'damaged' (occupied), the bond between them is also necessarily 'damaged'.

2. The model

In our model, we consider a number, $C_I L^2$, of particles that are randomly placed in the sites of the square lattice of side L. These particles move to a randomly chosen neighbour of the site they are occupying, with the restriction that they cannot immediately return to the previous site; on the square lattice the particle has three possible directions of motion. The sites visited by the particles become occupied. The fraction of occupied sites, q, is a measure of the time elapsed. The particles annihilate and disappear from the lattice when they visit occupied sites. Two neighbouring occupied sites are considered to belong to the same cluster. This is a connectivity criteria different from that used in kinetic gelation models where sites belong to the same cluster if there is a path of bonds linking them. Our model is not characterized by the functionality of monomers as in kinetic gelation. Every site of the lattice can be considered a monomer that is, in principle, able to make bonds up to the maximum number allowed by the geometry of the lattice, i.e. four bonds. However, the number of sites that have the four bonds occupied is small since this situation occurs only if two particles meet in a site already occupied.

With the bond connectivity criteria, our model can be related to a crack propagation model proposed by Nishiuma and co-workers [4]. In this case, the bond occupation is driven by the random motion of walkers, which try to avoid intersection with their own trajectories, following a type of random walk motion known as kinetic growth walk [6]. However, the formation of an infinite cluster (gel) in these kind of models [4], with the bond connectivity criteria, is not observed and the models are not interesting as gelation models. In our model, the walkers are of a self-avoiding type generated by sampling non-reversing random walks that terminate when a blind move leads the walker to a previously visited site [1, 6].

3. Results for critical parameters and critical exponents

We have studied systems of sides between 64, 128, 256, 512, 1024 and 2048. For systems with $L < 2048$ we considered at least 2000 and 1000 samples for systems with $L = 2048$. If the concentration of particles, C_I, is small all particles annihilate before an infinite cluster is found in the system. So, we have divided our study into two cases: in case A, we have measured the critical concentration C_I^* and we have studied the critical behaviour as a function of C_I, letting the system evolve until all the particles disappear; in case B, we have studied the time evolution of the system and the corresponding critical behaviour as a function of the fraction of occupied sites, q, for different initial concentrations, $C_I \geqslant C_I^*$.

We have measured the fraction of percolative samples, R, the fraction of sites in the infinite cluster, P_∞, and the mean cluster size (susceptibility), χ. We have considered a sample as percolative when there is a cluster that spans the lattice in one of the two directions. From the intersection of the R curves measured for systems of different sizes, L, we have estimated the critical parameter values for the infinite system. Since R follows the finite-size scaling law, $R \sim \Phi\big((x - x^*)L^{1/\nu}\big)$, with a scaling function $\Phi(y)$, its derivative with respect to the parameters C_I (case A) or q (case B) is expected to have a finite-size behaviour,

$$\frac{\mathrm{d}R}{\mathrm{d}x} \sim L^{1/\nu}\Phi'\left((x - x^*)L^{1/\nu}\right) \tag{1}$$

where x represents either C_I or q. Having estimated the critical parameter x^*, we have obtained the critical exponent ν from

$$\left(\frac{\mathrm{d}R}{\mathrm{d}x}\right)_{x^*} \sim L^{1/\nu}. \tag{2}$$

The system size behaviour of P_∞ at criticality

$$P_\infty \sim L^{-\beta/\nu} \tag{3}$$

was used to make estimations of the exponent $\frac{\beta}{\nu}$. The corresponding finite-size behaviour of the mean cluster size at criticality

$$\chi \sim L^{\gamma/\nu} \tag{4}$$

gives the exponent $\frac{\gamma}{\nu}$ [6].

3.1. Case A

The intersection values for the various $R(C_I, L)$ curves are presented in table 1 and lead us to the critical value of $0.098\,82 \pm 0.0002$. Starting with this critical value and according to equation (2) we obtain $\nu = 1.41 \pm 0.02$ (see figure 1). From the log–log plots of P_∞ versus L (figure 2) and χ versus L (figure 3), using equations (3) and (4), we obtain $\frac{\beta}{\nu} = 0.1031 \pm 4 \times 10^{-4}$ and $\frac{\gamma}{\nu} = 1.76 \pm 0.01$. These results are listed in table 2.

3.2. Case B

For this case we used the following initial particle concentrations: C_I^*, 0.2, 0.3, 0.45 and 0.5927 (close to the critical fraction of occupied site values in a 2D square lattice percolation [6]). The critical fraction of occupied sites, for each C_I, denoted by $q^*(C_I)$, is determined from the mean values of the intersection of the $R(q, L)$ curves (see table 1) for different system sizes. The measured critical exponents are presented in table 3. Figure 1 shows the log–log plot corresponding to equation (2) that allows us to measure ν. Figures 2 and 3 show the plots corresponding to P_∞ and χ that allow us to obtain $\frac{\beta}{\nu}$ and $\frac{\gamma}{\nu}$ according to equations (3) and (4), respectively.

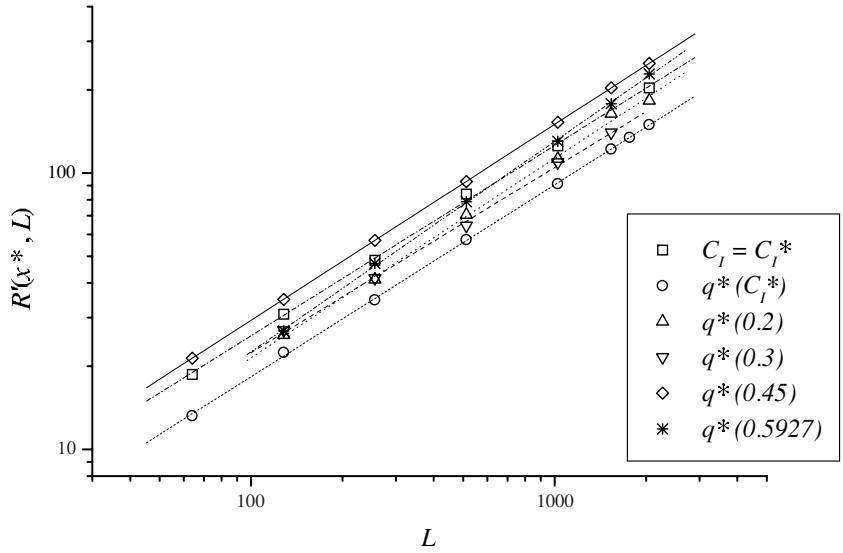

Figure 1. $(\frac{dR}{dx})_{x=x^*}$ versus L for cases A and B in log–log scale.

Table 1. Intersection points, x^*, of $R(x, L)$ curves for all system sizes studied, L, with $R(x, L')$ curves for the two largest systems, L'. In case A x is C_I and in case B x is q.

Case	L'/L	64	128	256	512	1024	1536
A	1024	0.098 90	0.098 87	0.099 00	0.099 02		
	2048	0.098 82	0.098 79	0.098 81	0.098 79	0.098 68	
B, $C_I = C_I^*$	1765	0.4678	0.4677	0.4678	0.4678	0.4679	0.4679
	2048	0.4674	0.4673	0.4673	0.4672	0.4671	0.4675
B, $C_I = 0.2$	1536		0.5181	0.5181	0.5182	0.5181	
	2048		0.5179	0.5177	0.5175	0.5174	0.5169
B, $C_I = 0.3$	1024		0.5425	0.5421	0.5421		
	1536		0.5427	0.5421	0.5422	0.5436	
B, $C_I = 0.45$	1536	0.5708	0.5708	0.5809	0.5712	0.5708	
	2048	0.5702	0.5702	0.5702	0.5702	0.5697	

4. Phase diagram

Since at $t = 0$ we have $q = C_I$, we obviously have $q > C_I$ at any time. Furthermore, we can define a maximum value of q for each C_I, $q_{\max}(C_I)$, representing the maximum fraction of occupied sites that we can obtain after the annihilation of all the particles. Therefore, in the C_I–q plane, we can define a forbidden region and an accessible region delimited by the straight line $q = C_I$ and by the curve $q = q_{\max}(C_I)$ obtained from numerical simulations. The accessible region is divided into two regions separated by a line of critical points. This line connects, in the C_I–q plane, the point $(C_I^*, q^*(C_I^*))$ with the point $(q_{per}^*, q^*(q_{per}^*))$ where $q_{per}^* = q^*(q_{per}^*) = 0.5927\ldots$. For $C_I = q_{per}^*$, we already have at $t = 0$ a percolative cluster and the subsequent site occupation leads us away from criticality. We now present an argument for the functional dependence $q^*(C_I)$: the geometrical phase transition for a value C_I occurs at some q^* such that the mean linear size of the clusters originated by the motion of a given

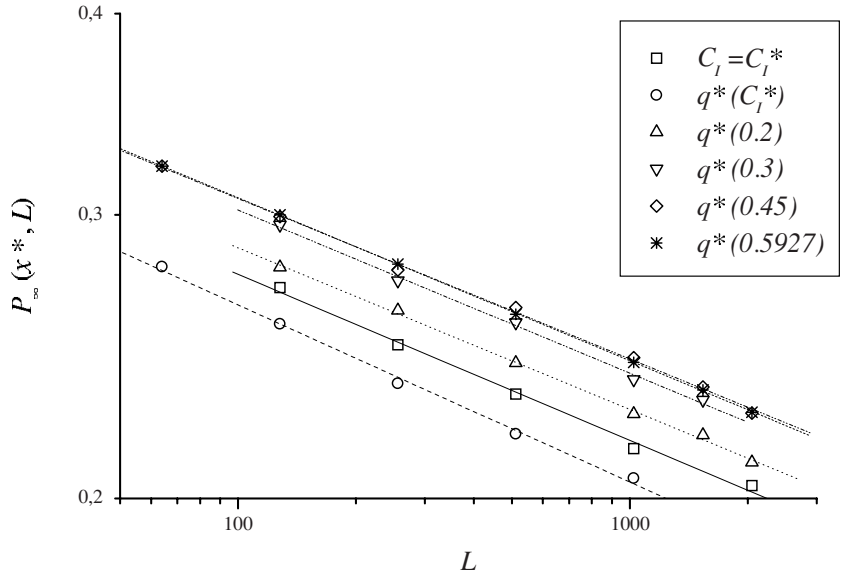

Figure 2. P_∞ versus L for cases A and B in log–log scale.

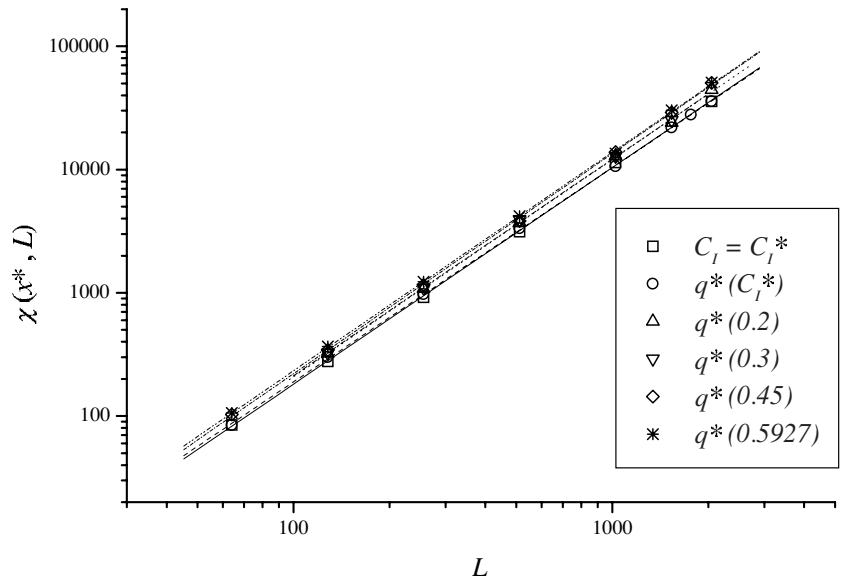

Figure 3. χ versus L for cases A and B in log–log scale.

particle is of the same order as the mean distance between them. The mean number of sites visited by one particle is of the order of $\frac{q}{C_I}$. Supposing that the cluster formed by the random walk of each particle is a fractal with fractal dimension, d'_f, then the cluster mean linear size is of the order of $\left(\frac{q}{C_I}\right)^{1/d'_f}$. Since the mean distance between clusters is $(C_I)^{-1/2}$, we have an infinite cluster when $\left(\frac{q}{C_I}\right)^{1/d'_f} = (C_I)^{-1/2}$, i.e.

$$q^* \sim (C_I)^{1-d'_f/2}. \tag{5}$$

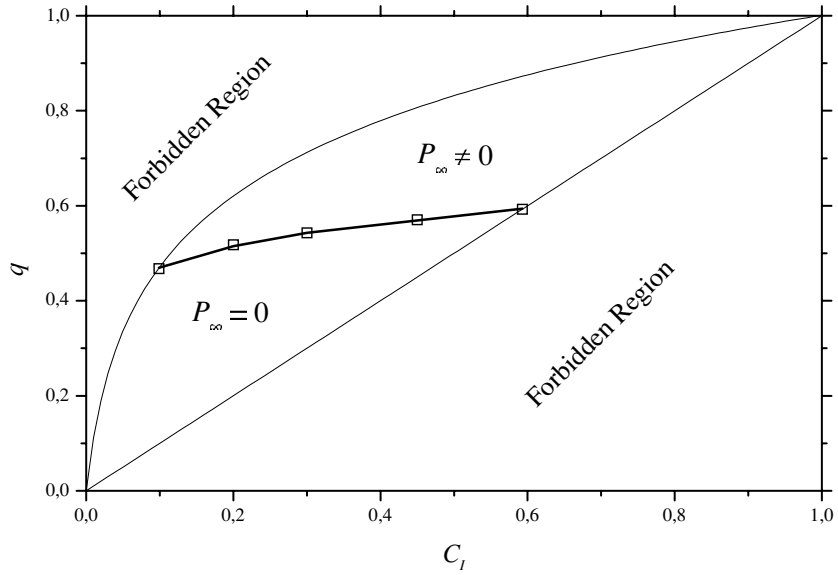

Figure 4. Phase diagram in the C_{I-q} plane.

Table 2. Critical particle concentration and measured critical exponents for case A.

C_I^*	ν	$\frac{\beta}{\nu}$	$\frac{\gamma}{\nu}$
$0.098\,82 \pm 2 \times 10^{-4}$	1.41 ± 0.02	$0.1031 \pm 4 \times 10^{-4}$	1.76 ± 0.01

Table 3. Critical fraction of occupied sites and critical exponents for case B with $C_I = C_I^*$, 0.2, 0.3, 0.45 and 0.5927.

C_I	q^*	ν	$\frac{\beta}{\nu}$	$\frac{\gamma}{\nu}$
C_I^*	$0.4679 \pm 5 \times 10^{-4}$	1.42 ± 0.02	$0.110 \pm 4 \times 10^{-3}$	1.74 ± 0.02
0.2	$0.5179 \pm 3 \times 10^{-4}$	1.40 ± 0.02	$0.100 \pm 2 \times 10^{-3}$	1.76 ± 0.02
0.3	$0.5431 \pm 7 \times 10^{-4}$	1.41 ± 0.02	$0.101 \pm 3 \times 10^{-3}$	1.76 ± 0.02
0.45	$0.5705 \pm 3 \times 10^{-4}$	1.41 ± 0.02	$0.100 \pm 3 \times 10^{-3}$	1.77 ± 0.02
0.5927	$0.5927^{(\text{assumed})}$	1.32 ± 0.02	$0.101 \pm 3 \times 10^{-3}$	1.76 ± 0.02

With the values obtained for $q^*(C_I)$ and with the value corresponding to the critical parameter of 2D site percolation, we have determined for d'_f the value 1.74. The C_I–q phase diagram is presented in figure 4.

5. Discussion

We have obtained values for ν near 1.4, from both cases A and B, for all initial particle concentrations, except for the case with $C_I = q^* = 0.5927$, the 2D site percolation critical parameter. The value of 1.4 is consistently larger than the 2D percolation value known to be 4/3. On the other hand, for $C_I = q^*_{per}$ the value obtained for ν is rather close to this percolation value. The measured ratios of the exponents, β/ν and γ/ν, are always close to the 2D percolation ratios $\frac{5}{48} = 0.104\ldots$ and $\frac{43}{24} = 1.79\ldots$ [6]. The errors estimated in the determination of ν from the finite-size behaviour of $\frac{\mathrm{d}R}{\mathrm{d}x}$ could be underestimated and it is

possible that the consideration of larger systems, for which finite-size corrections would be smaller, would lead us to values of ν consistent with percolation. So we prefer to consider the ν values reported as effective exponents. However, for $C_I = q^*_{perc}$, the results obtained for ν, assuming the known critical value 0.5927 . . . , lead us to a ν value very close to the percolation value in spite of the fact that the system sizes of the systems studied were the same as in the previous cases.

The behaviour of the line of critical points in the plane C_I–q was predicted from an approximate argument. The value obtained for d'_f was smaller than the value of the infinite cluster fractal dimension of 2D percolation known to be $\frac{91}{48} \simeq 1.896$ [7]. This difference could be attributed to the fact that the cluster structures, originating from the motion of a particular particle, have an intrinsic fractal dimension different from the infinite cluster formed by the clustering of these clusters. Actually, the walks originating from each particle can be seen as self-avoiding walks generated by simple random walks that have a survival probability decaying exponentially with the number of steps (visited sites). For long self-avoiding walks, it is known that $d_f = 4/3$ [1], which is smaller than the measured value of 1.74. However, in our model the walks are not long enough for the asymptotic properties to be seen and so a large effective fractal dimension is expected. Finally, we mention that the ratio β/ν which we obtain is always near the 2D percolation value which means that the infinite percolative cluster in our model has the same fractal dimensions as 2D percolation.

6. Conclusions

In this paper, we have presented the numerical study of a new growth model of structures, related to kinetic gelation models. In our model we use site connectivity criteria instead of the bond connectivity used in gelation models. Furthermore, the mechanism for the growth of structures is different than that considered in gelation models; the motion of the particles (the initiator agents in gelation) are not determined by a given functionality of monomers in the system and they annihilate when they visit occupied sites. Our model, with the bond connectivity criteria, does not show any critical behaviour whatever the initial concentration of particles we start with [4].

We have made a static study (case A) where we wait for all particles to annihilate. In this case, there is a critical initial concentration of particles. The kinetic study, case B, was done for initial particle concentration larger than the critical concentration determined in case A. In this case we measure the fraction of occupied sites and study the critical behaviour arising when a percolative infinite cluster appears in the system. We were able to characterize the phase diagram of the model in the C_I–q plane where there is a line of critical points behaving like $q^* \sim (C_I)^{1-d'_f/2}$. The fractal dimension d'_f measured is different from the fractal dimension of the infinite percolative cluster.

The effective critical exponent ν measured was always larger than the 2D percolation value, close to 1.4 for all critical points studied except for the critical point corresponding to $C_I = q^*_{perc}$ where the result for 2D percolation was found. The ratios of exponents β/ν and γ/ν are, in all cases, consistent with the 2D percolation exponents.

Finally, we mention that our model could be related to reaction-diffusion models that can be studied by field-theoretic techniques [8, 9]. In particular, Cardy and Grassberger [9] have shown that a model of random walkers with poisoning of visited sites and offspring birth belongs to the percolation universality class. In our model, offspring birth processes are not included and it is not possible to build an infinite percolative cluster starting with a single particle as is possible in epidemic models [1] such as those studied by Cardy and Grassberger [9].

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