

Variation of the critical percolation threshold with the method of preparation of the system

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Abstract. In the present work we propose a model in which one may vary at will the critical threshold p_c of the percolation transition, by probing one candidate site (or bond) at a time. This is realised by implementing an attractive (repulsive) rule when building up the lattice, so that newly added sites are either attracted or repelled by the already existing clusters. We use a tuning parameter k , which is the number of attempts for a site to be occupied, leading to a continuous change of the percolation threshold while the new percolation process still belongs to the same universality class as the ordinary random percolation. We find that by increasing the value of the tuning parameter k , p_c decreases until it reaches a minimum value where nucleation effects are now more pronounced than the percolation process. Such results are useful for the explanation of several new experimental systems that have recently appeared.

1 Introduction

The percolation phase transition [1] has traditionally attracted the interest not only of physicists, but of scientists in practically all fields over the last five decades due to the fact that it is a paradigmatic continuous phase transition. Percolation models are used not only for their theoretical interest, but also because many physical and chemical processes can be simulated using percolation theory, for example characterisation of porous media, earthquake, fracture and fault patterns, hydrodynamic behaviour in ground water flow, and several more [2]. Additionally, besides the basic simple model, several different variations have been developed in recent years because of different ways that experimental systems are prepared. This may lead to different threshold values, and different characteristics of the phase transition, including the question of whether the transition is continuous or discontinuous.

We already know that different underlying lattices have different percolation thresholds and furthermore, we know that by varying the percolation process one can also obtain phase transitions with not only different thresholds but also with different characteristics, such as different universality properties. The explosive character of the percolation transition [3] has recently succeeded in capturing the interest of the scientific community in the corresponding field. The initial idea included a 2-particle probe method, which caused the critical point to be considerably delayed. Thus, for a square 2D lattice the critical

point moved from $p_c = 0.593$ to $p_c = 0.755$. This is due to the fact that the probe method introduced by Achlioptas et al. takes into account global information of the system and strongly depends on the pre-existing system structure. We use the same idea as the original Achlioptas probe method, but instead of choosing the site that results in the smaller product or sum of the joining cluster we now choose exactly the opposite, i.e. we choose to keep the probe site which results in the largest cluster and we discard the other probe site. In the original model one fills the system (lattice or network) by probing at random two candidate sites (or nodes) to be occupied. We maintain the one that minimizes the product of the sizes of the clusters to which this site is about to connect, while the other one is removed. The details for candidate sites maybe different depending on the system used [3–5]. For example, in site percolation in a two-dimensional (2D) square lattice there is a maximum of four possible clusters that can be merged, while in the original Achlioptas processes the newly added bond may connect only two clusters to form a larger one. However, such details do not affect the overall system behaviour. Obviously, this will result in a speed-up of the critical point, i.e. the largest percolating cluster will now appear earlier than in the conventional case. Indeed we find that instead of $p_c = 0.593$ we now have $p_c = 0.531$. Thus, the speed-up of the critical point gives the complementary case of the celebrated Achlioptas model.

A similar behaviour can be seen in different lattice geometries and dimensionalities, as well as in networks, where the critical point refers now to the creation of the largest network component. Recent applications of the

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newly developed models include work where the properties of a single-walled nanotube bundle with uniform diameter have been examined [6]. Another case refers to real-world networks of scientific collaboration network [7], and another is concerned with mobile telephone calls network [8]. Biological applications include the emergence of a spanning cluster in the human protein homology network, which has features similar to a more abrupt transition and is markedly different from the classical case of random percolation [9]. The above list is not exhaustive but shows that the initial percolation model has historically advanced to new directions, requiring new theoretical approaches and new models.

The delay in achieving criticality in the percolation problem introduced in reference [3] has certainly attracted considerable interest in recent years because it gives one a method to vary the exact location of the critical point. Following this, a plethora of scientific works have been published introducing variations of percolation phase transitions by appropriately handling the conditions by which the system is being built up or prepared [10–13].

The symmetrical case to the delay of criticality can be achieved for the equivalent speed-up, by using an opposite process. Recently, we showed [14] that by using a different number of probe sites one can further vary to a considerable extent the location of the critical point, showing a well-behaved monotonic behaviour of the location of the critical point as a function of the number of probe sites. The question of how percolation systems depend on the number of probe links has been studied on networks [15,16] and on lattices [17–19]. In reference [15] Nagler et al. working on Achlioptas processes showed how the competitive addition of single links may drastically change the macroscopic connectivity in networks, and in reference [16] Riordan and Warnke explained that all Achlioptas processes have continuous phase transitions. In reference [17] the authors studied a variant of the percolation process in lattices and arrived at the tricritical crossover exponent, while in reference [18] Cho et al. showed that in the thermodynamic limit the phase transition can be either continuous or discontinuous depending on a control parameter. Other works on lattices, such as [19] have investigated the conductivity behaviour through a discontinuous bond percolation model evolving under a suppressive external bias. These findings showed that the conductivity function exhibits a smoothly increasing function beyond the percolation threshold in the thermodynamic limit.

In a recent experiment [20–24] it has been found that carbon nanotubes merging into clusters do not follow random placement, but are amenable to an attractive field, which cannot be explained by classical means. Towards this direction, we introduce a different model for probing sites in a percolating system and we also introduce an attractive field. We do this by adding only one site at a time using a simple and reversible rule. Initially we choose at random a site in a two dimensional lattice and we investigate its nearest neighbourhood (the four nearest neighbours of the chosen site). Then we decide to occupy it only if it has at least one occupied nearest neighbour. The

newly added site is being attracted by its neighbour. If the randomly chosen site has no neighbours at all then we decide not to occupy it. In this case we randomly choose another site and we occupy it regardless of the number of its neighbours. This procedure promotes the attraction between nearest sites and for this reason large clusters merge faster than in the classical percolation case. This attracting process results again in the early emergence of the percolation threshold as largest clusters attract any newly added site in the system with higher probability. We find this speed-up in criticality produces a critical point p_c that may have value close to $p_c = 0.5$ instead of $p_c = 0.593$. We have also evaluated the opposite process by promoting the isolated sites and suppressing the emergence of large clusters. In this case sites with no occupied neighbour are preferred, and as expected a delay to criticality occurs. The critical point now rises to $p_c = 0.610$. This method tunes the critical point below and above the one of classical percolation transition, which results in a behaviour similar to the Achlioptas processes. Similarly, we calculate the opposite process of [3], leading to the speed-up of the appearance of the critical point, in order to compare the two models.

Due to recent experiments mentioned earlier [6–9,20–24], in principle, one could design a percolation system with various critical threshold values, by appropriately varying the number of attempts. The idea described earlier constitutes one attempt ($k = 1$), while we may vary the value of k (to any integer or non-integer value) until we get a system with the desired critical percolation threshold. Here we find that with a single parameter (the number of attempts k), the percolation threshold p_c goes through a minimum. Thus, one can vary the location of the critical point in percolation systems at will by choosing only one candidate site (bond) at a given time and by varying just one parameter (k). The models proposed in this work are important when preparing a new system with a specifically needed percolation threshold. Because of the variation of the underlying lattice one can only extract a certain number of discrete critical values which are unique for each topology, while in our model, tuning the parameter k can result in continuous critical values.

2 Model description

We introduce two models, which are based on filling the lattice by probing the local environment of the site to be added; one using an attractive algorithm, and one using a repulsive one. In the attraction model we start initially with an empty 2D square lattice of linear size $L = 1000$ sites. We start by probing one site of the lattice at random and we occupy it only if this site has at least one neighbour occupied. We consider that each site has four nearest neighbours. If the chosen site has no nearest neighbours occupied, we then choose at random another site of the lattice without investigating whether or not there are any occupied neighbours (random site percolation) and we occupy it. We continue by probing a second

site, and so on, and we repeat the same process as previously described. In the repulsion model we start again with an empty 2D square lattice of the same linear size $L = 1000$ sites and we probe a site at random. We then investigate the four sites that neighbour the candidate site and we occupy the candidate site only if no neighbours are occupied. On the other hand, if there is at least one neighbour site that is occupied, we choose another site at random and we occupy it. For both the attraction model and repulsion model we continue until the lattice is fully occupied.

We investigate four variations of the well known Achlioptas processes [3]. We have reproduced the data for site percolation product-rule and sum-rule and our results are in excellent agreement with previous publications [4,5]. Here we extend both these models by promoting the creation of larger clusters instead of smaller ones. In order to do this we first choose two candidate sites. We calculate the product of the sizes of the clusters that are to be merged for each candidate site separately. Then we keep the site with the larger of the two products while we discard the other one. This results in the critical point appearing earlier than in normal percolation. Thus, in addition to the delay of criticality that was suggested by the Achlioptas models, one may now speed-up the appearance of the critical point.

These two models, the attraction and the repulsion model, are expected to significantly change the location of the critical point, which can conceivably be further changed. This can be done by increasing the number of attempts, for both the attraction and the repulsion models, which is expected to increase the level of speed-up or delay of the critical point, respectively. To investigate this we consider the same 2D square lattice of linear size $L = 1000$ sites, but this time we introduce a parameter k which is the number of attempts we apply until we find a site which verifies the attractive rule or the repulsive one, respectively. Thus, for $k = 0$ this corresponds to conventional random site percolation. $k = 1$ gives the model explained in the previous paragraph, where we have only one attempt to search for occupied nearest neighbours before we probe a site of the lattice at random. $k = 2$ results in two independent attempts. More specifically, in the attraction model we start again with an empty lattice and we probe at random a site to be occupied. If this chosen site has no nearest neighbours occupied, we probe another site at random and we investigate again for occupied nearest neighbours. That was the second attempt ($k = 2$). If again no nearest neighbours are occupied we occupy a random site in the lattice without checking its neighbours. It is important to mention that if we find a nearest neighbour occupied during the attempts, the process stops and a new Monte Carlo step starts from the beginning. This procedure can be extended to larger k values, and in principle, even to non integer values. This is done, for example, by using in one step $k = 1$, while using $k = 2$ in the next step, and subsequently alternating these two values. We report simulations with different k values for both the attraction and the repulsion models.

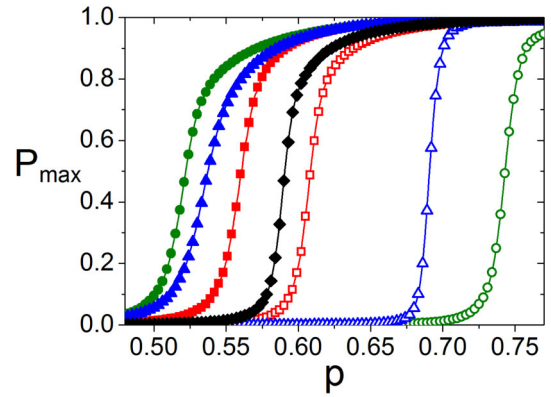


Fig. 1. Plot of percolation strength (P_{max}) as a function of the density of occupied sites p for a 2D square lattice of linear size $L = 1000$ for classical random site percolation (\blacklozenge), attraction model ($k = 1$) (\blacksquare), repulsion model ($k = 1$) (\square). Sum-rule for the delay of criticality (\triangle), sum-rule for the speed-up version (\blacktriangle). Product-rule for the delay of criticality (\circ), and product-rule for the speed-up version (\bullet). The lines are optical guides.

3 Results

We monitor the percolation strength P_{max} , which is the probability of a given occupied site belonging to the largest percolating cluster. P_{max} is in the range $0 < P_{max} < 1$ and it represents that part of the system that has been occupied by the percolating cluster. Equation (1) gives P_{max} as a function of the density of occupied sites p

$$P_{max} = \frac{S_1}{pL^2}, \quad (1)$$

where S_1 is the size (number of sites) of the largest cluster of the system at density p , and L^2 is the total number of lattice sites.

In Figure 1 we give P_{max} for seven different models. These are the curves for attraction and repulsion methods compared with the product and sum rule of Achlioptas processes. We also plot the cases of enhancing the critical point of product and sum rules (reverse processes) in order to compare them with the attraction model which speeds-up the appearance of the spanning cluster. The classical site percolation threshold is $p_c = 0.593$ (full diamonds). The Achlioptas product (PR) and sum-rule (SR) for the delay of criticality are shown with $p_c = 0.755$ (open circles) for PR, $p_c = 0.694$ (open triangles) for SR. The equivalent Achlioptas processes for the early emergence of criticality now produce $p_c = 0.531$ (full circles) for PR, $p_c = 0.543$ (full triangles) for SR. The critical threshold for the attraction model is $p_c = 0.562$ (red full squares) and for the repulsive model is $p_c = 0.610$ (red empty squares). The values of these critical points can be deduced from Figure 1 as the inflection point of the s-shaped curve. This point is usually found in the middle of the steep rise of the corresponding curve. In order to evaluate as accurately as possible the position of the inflection point from Figure 1, one can investigate the first derivative of P_{max} . We thus, calculate $\frac{dP_{max}}{dp}$ for all seven cases, and we show

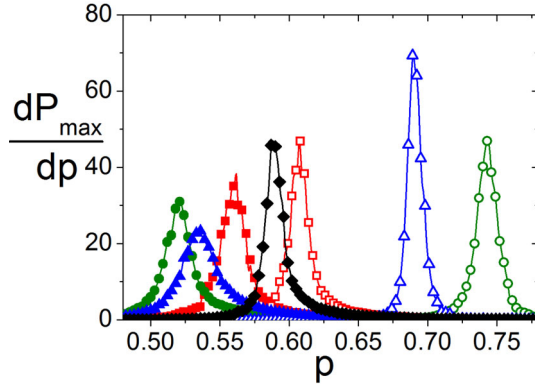


Fig. 2. Plot of the first derivative ($\frac{P_{max}}{dp}$) of percolation strength as a function of the density of occupied sites p for a 2D square lattice of linear size $L = 1000$ for classical random site percolation (\blacklozenge), attraction model ($k = 1$) (\blacksquare), repulsion model ($k = 1$) (\square). Sum-rule for the delay of criticality (\triangle), sum-rule for the speed-up version (\blacktriangle). Product-rule for the delay of criticality (\circ), and product-rule for the speed-up version (\bullet). The lines are optical guides.

the results in Figure 2. We observe that the peak of the curvature of the first derivative gives the critical density p_c for each model. The values of p_c for direct product-rule and sum-rule as well as for the classical percolation are in excellent agreement with previous publications [1,4,5,25], while values for critical densities for the reverse processes of product and sum-rule are now calculated here.

Table 1 illustrates the critical threshold for all seven different models that are included in Figures 1 and 2. Furthermore, we investigate the universality class of our new continuous methods. The universality property is a general property of second order phase transitions, where the order parameter (here it is the size of the infinite cluster S_1) introduces an abrupt increase at the region near the critical point. We calculate the universal critical exponent which does not depend on the structural details (topology) of the lattice or on the type of percolation (site, bond). This exponent is the fractal dimension d_f . We also calculate the correlation length critical exponent $\frac{1}{\nu}$. The two exponents are uncorrelated and their calculation enables us to define the universality class to which they belong. We use the Finite Size Scaling property to extract this information. In addition, we use a novel method that we have recently published [26] and it concerns the estimation of the critical quantities ($p_c, \frac{d_f}{\nu}, \frac{1}{\nu}$) via a minimization procedure requiring low statistical sampling for the determination of the universality class. The results are shown in Table 1.

Equation (2) shows the logarithmic relation of S_1 to the linear size of the lattice L around the critical point ($p \approx p_c$)

$$S_1(L)_{(p \approx p_c)} \sim L^{d_f}. \quad (2)$$

In order to calculate the correlation length critical exponent $\frac{1}{\nu}$, we can use the scaling relation shown in equation (3). It is known [1] that for the infinite system ($L \rightarrow \infty$), the difference for each L , $p_c(L) - p_c$, scales

Table 1. The critical percolation threshold p_c and the critical exponents d_f and $\frac{1}{\nu}$ for all seven models simulated in this work. The results are for site percolation transition on a 2D square lattice.

Model	p_c	d_f	$\frac{1}{\nu}$
Classical percolation [1]	0.5927	1.8954	0.75
Attraction model ($k = 1$)	0.5618	1.89 ± 0.02	0.75 ± 0.02
Repulsion model ($k = 1$)	0.6100	1.89 ± 0.02	0.75 ± 0.02
Product rule (delay)	0.7554	1.98 ± 0.02	0.95 ± 0.02
Product rule (early emergence)	0.5315	1.89 ± 0.02	0.76 ± 0.02
Sum rule (delay)	0.6942	1.99 ± 0.02	0.96 ± 0.02
Sum rule (early emergence)	0.5433	1.88 ± 0.02	0.74 ± 0.02

with the system size as a power law function. Equation (3) illustrates this logarithmic relation

$$|p_c(L) - p_c| \sim L^{\frac{1}{\nu}}. \quad (3)$$

In order to identify both critical exponents d_f and $\frac{1}{\nu}$ from the scaling relations (2) and (3) one can assume the existence of two independent fitting parameters, d_f and p_c for equation (2), and $\frac{1}{\nu}$ and p_c for equation (3). This power-law relation can be verified by tuning p_c until a straight line appears, as shown in Figure 3. The specific values of p_c and d_f or $\frac{1}{\nu}$ which correspond to straight lines in Figures 3a and 3b are the resulting values for those quantities.

Figure 3a illustrates the scaling of the size of the largest cluster at the critical point $S_1(p = p_c)$ as a function of L . The slope of the straight line gives the fractal dimension d_f , which for the classical random percolation is well-known, and its value has been calculated ($d_f \approx 1.8954$) [1]. We observe that the slopes of the three straight lines in Figure 3a have the same value ($d_f = 1.89 \pm 0.02$). We observe the same behaviour in Figure 3b. The slopes of all three lines are almost identical ($\frac{1}{\nu} \approx 0.75$). This illustrates the fact that both the attraction and repulsion models belong to the same universality class with random percolation. In the present work we also extracted the critical exponents for all Achlioptas processes. The error bars are due to the unusual finite size behaviour of the critical exponents of this second order phase transition [27–29]. The results are shown in Table 1 and those which belong to the delay of criticality ensemble are in very good agreement with previous publications [4,5,25,27,30]. Results that refer to the early emergence of the critical point of Achlioptas processes have been newly calculated in the present work.

One can see an interesting observation in Figure 1 in that the curves for the attraction model and repulsion model are not symmetric around the curve for the classical percolation. This is due to the fact that the rule that we use is not exactly equivalent for both models. For very low densities ($p < 0.1$) the majority of the newly added sites are randomly distributed in the system for both models. There are many isolated sites and the majority of the

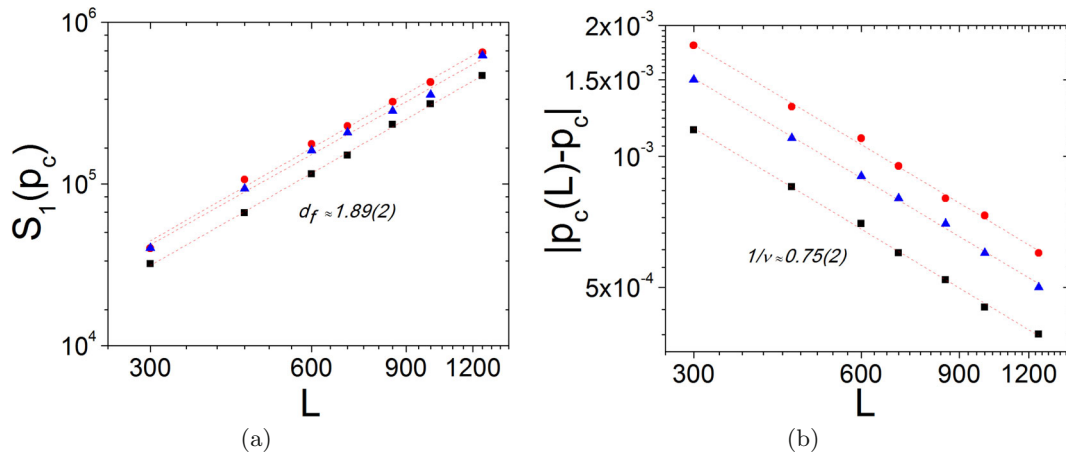


Fig. 3. Finite size scaling of the size of the largest cluster at the critical point $S_{1(p=p_c)}$ (a) and the difference between $p_c(L)$ and p_c (b) as a function of the linear lattice size L for the attraction (red circles) and the repulsion (blue triangles) models in log-log coordinates. Black squares are for the classical percolation case. The slopes of the straight lines give the fractal dimension d_f and the correlation length critical exponent $\frac{1}{\nu}$ respectively. All curves at each plot have similar slopes, meaning that these models belong to the same universality class.

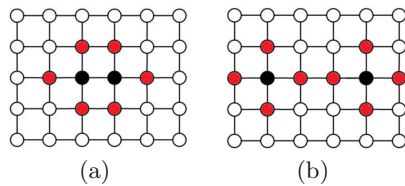


Fig. 4. The difference in the construction process between attraction model (a) and repulsion model (b). White sites are empty, black sites are occupied, whilst red ones are those with at least one occupied nearest neighbour. There are more red sites for a fixed number of black sites in the repulsion model.

system consists of empty space. In the attraction model the newly chosen site is isolated most of the time and thus, a new site is chosen to be occupied (random percolation). In the repulsion model again we chose at random to occupy a site. Since it is more probable that there are no occupied nearest neighbours, we occupy this specific site, which at these low values of p , occurs most frequently in almost every Monte Carlo step. Again, this procedure is equivalent to random percolation. At higher density values but still lower than the critical, ($0.1 < p < 0.5$), in the attraction model the system consists of small clusters. In contrast, in the repulsion model the system is sparse (the majority of occupied sites is isolated). As a result, when we choose to occupy a site at random, in the attraction model this site is attached to the clusters that already exist in the system, while in the repulsion model, it is more likely for each randomly probed site to have an occupied nearest neighbour, and thus a new site is chosen at random. This process leads to the random percolation process. In Figure 4 we give a schematic of a lattice, where one can easily see that for two occupied sites (black) there are six sites with at least one occupied neighbour (red) in the

attraction model (left panel), while there are 8 of them in the repulsion model (right panel). As a result, for a given density of occupied sites p , there is a higher probability of having random percolation in the repulsion model than in the attraction model. In higher densities ($0.5 < p < 1$) the system undergoes a phase transition and the majority of sites are occupied. In this last state there are only a few sites that are not occupied and the number of those which are isolated (no nearest neighbours) becomes even smaller. Thus, almost each new randomly chosen site is directly occupied in the attraction model because newly added sites are attracted by occupied neighbours. However, in the repulsion model, since the number of isolated sites is almost zero, random percolation occurs again (because the probability of choosing an isolated site is very small). Thus, at this point, repulsion and attraction models are both equivalent to the well-known random percolation. The simulations (Fig. 1) and the qualitative approach (Fig. 4) show that the rule for the attraction model and the rule for the repulsion model are not exactly equivalent during the percolation transition process. This is the reason why the curves for these two models are not symmetric around the curve of classical random percolation. This asymmetry still exists even for k values higher than one (Fig. 5).

We obtain results with different k values for the attraction and repulsion models. We illustrate the results for both models in the same plot, in Figure 5 which shows the critical threshold p_c for both attraction and repulsion models and for different values of attempts k . We observe that there is a minimum p_c for the attraction model for $k \approx 15$. For $k > 15$ the speed-up for the attraction model does not have any further effect and further increase of the number of attempts k results again in higher values of the critical point p_c . The shape of the curve in Figure 5 with the minimum value for the delay of criticality,

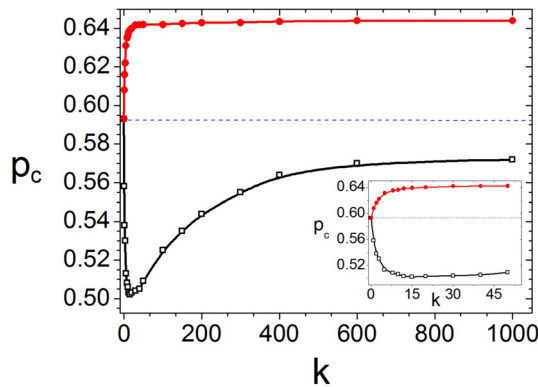


Fig. 5. The percolation threshold of sites p_c vs. the number of independent attempts k for attraction and repulsion models. The attraction model is illustrated with empty squares whilst the repulsion model is illustrated with full circles. The lines are only optical guides. The blue dashed line indicates p_c for classical percolation. In the inset: critical density of sites p_c vs. number of attempts k to indicate the minimum and the maximum of the two curves.

is quite unexpected, but it can be explained by the fact that after this minimum value the newly added sites are attracted to already existing clusters, with hardly any new clusters being formed. No new clusters appear (or the rate of appearance is limited). This is similar to crystallization starting from active centers. Thus, the formation of the infinite cluster which is spanning the entire system is delayed because there are a small number of clusters which are growing simultaneously and need more time to grow in all directions until they touch each other to form a larger one. In the limit of $k \rightarrow \infty$ there is only one nucleus that grows. The larger the k value, the stronger the similarity of the model to that of overall crystallization kinetics [31]. When a large number of attempts k are made most of the newly deposited sites are attached to the already existing clusters (except for the initial stages). In a sense, at this range the filling of the lattice is equivalent to a crystallization process, which proceeds from an initially small number of active centers.

4 Discussion and conclusions

In this work we have examined two different models of the percolation phase transition, which depend on the method used to fill the lattice sites. We used the direct and reverse models of the well-known Achlioptas processes, using both the product and the sum rule. The two new models are based on the local environment of the site to be added, by examining the occupancy of the nearest neighbours of the probing sites. The attraction model promotes the merging of sites to form larger clusters, whilst the repulsion model (which is the reverse process) promotes the isolation of occupied sites. We located the exact position of the critical density for all seven models that we have examined. We compared the new findings with well known results, and we found excellent agreement. Our results show that the

two new models belong to the same universality class as the classical percolation transition. The advantage of this method is that the new parameter k can now take not only integer values but it is a continuously varying parameter, effectively leading to continuously varying critical percolation threshold values. We explained the asymmetry that appears in the attraction and repulsion model around the normal critical transition point. The models proposed in this work can be implemented either in bond percolation in lattices or in networks. The impetus for this work has been the fact that one can vary the location of the critical point between a minimum and maximum value of the p range, by varying the values of the building parameters of the clusters. We find that the percolation threshold p_c goes through a minimum as k is increased. These results are very useful for several new experimental systems, which have appeared recently, showing different values for the percolation threshold. From Figure 5 one can conclude that there is a minimisation in the reduction of the value of the critical point, after which crystallization-like processes take place in the system resulting in a not so pronounced speed-up of the percolation process. This variation alone may also be important when preparing a new system with custom-made properties, which can now be tailor-made according to the required specifications.

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