A Monte Carlo analysis of percolation of line-segments on a square lattice.

Y. Leroyer and E. Pommiers

Laboratoire de Physique Théorique
CNRS, Unité Associée 764
Université de Bordeaux I
19 rue du Solarium, 33175 Gradignan Cedex, France

Abstract

We study the percolative properties of bi-dimensional systems generated by a random sequential adsorption of line-segments on a square lattice. As the segment length grows, the percolation threshold decreases, goes through a minimum and then increases slowly for large segments. We explain this non-monotonic behaviour by a structural change of the percolation clusters. Moreover, it is strongly suggested that these systems do not belong to the universality class of random site percolation.

LPTB 93-21
December 1993
PACS 05.70Ln, 64.60Ak
e-mail : Leroyer@frccp11.in2p3.fr
1 Introduction

The random site percolation model has been extensively studied [1, 2] and some exact results have been obtained concerning the geometrical phase transition that this system undergoes. For most real percolating systems, the particles are extended objects, more or less isotropic, and some of their physical properties depend on the detailed geometry of the particles. These systems form a larger class of models, the correlated site percolation model. On the basis of renormalisation-group arguments, it is believed that, as long as the sites are correlated on a finite range, the universal properties of these systems are described by the random site percolation critical point. [1, 2, 3, 4, 5] However, some non-universal parameters, such as the percolation threshold, are of physical interest, and their determination provides useful information on the system. Among the many authors who have investigated the various aspects of the discrete or continuous versions of this model, let us cite the comprehensive numerical work of Pike and Seager [7] on the continuous percolation problem for various extended objects.

One of these systems, the percolation of rod-like objects, has received much attention due to its connection with composite materials made of conducting fibers embedded in an insulating resin [3, 4, 5]. The percolation transition is linked to the metal-insulator transition, and the critical concentration is an important parameter which characterises the properties of the material. Alternatively, the same system restricted to two dimensions, can describe the adsorption of conducting rod-like polymers on a silicon substrate on which active sites are regularly disposed [6]. These systems involve very asymmetric objects, and the excluded volume effect, which drives the
deposition process, strongly influence the geometry of the percolative configurations, especially in two dimensions, and consequently, may affect the non-universal as well as the universal properties of the system.

In this paper, we investigate this system in the framework of a Monte-Carlo analysis of a two-dimensional lattice model, where the rod-like objects are simulated by line segments and the configurations are generated by a random sequential adsorption process with hard core exclusion. In the next section, we present the technical details of the Monte-Carlo simulation, and the determination of the percolation threshold as a function of the segment length. The third section is devoted to a test of the universality of this system, and we expose our conclusions in the last section.

2 The percolation threshold

The model that we investigate in this paper, is defined as follows: the substrate is a square periodic lattice of linear size $L$ on which we drop a line segment which covers exactly $k$ sites, aligned along one of the lattice axes, and such that the segment sites exactly fit the lattice. It sticks if it doesn’t overlap previously deposited segments, otherwise it is rejected. The process is repeated, and the density of the configurations increases, until percolation occurs: we say that the system percolates when there is a connected path of occupied sites which spans the lattice either horizontally or vertically (rule $R_0$ of ref. [10]). We denote by $p_c(L)$ the critical concentration, averaged over a sample of $N_S$ percolating configurations (we take $N_S$ in the range $(100, 500)$). So defined, the finite size percolation threshold $p_c(L)$ corresponds to
the $p_{av}$ of ref. [1] or $\langle p \rangle$ of ref. [10], i.e.

$$p_c(L) = \int_0^1 \frac{dR_L}{dp} p\, dp$$

where $\frac{dR_L}{dp} dp$ is the probability for a system of size $L$ to percolate at a density in the range $(p, p + dp)$.

For each segment length $k$, we have measured $p_c(L)$ for several (6 to 8) increasing lattice sizes $L$ up to a value $L_{max}$ such that $25k \leq L_{max} \leq 1024$. We show in Table I a significant subset of our results, where the error bars for finite $L$ are statistical.

We then perform the $L \to \infty$ extrapolation by means of the finite size scaling law:

$$p_c = p_c(L) - AL^{-\omega}$$

If the transition belongs to the random site percolation universality class, the exponent $\omega$ is linked to the exponent $\nu = 3/4$ of the correlation length: on the basis of the renormalisation-group, one expects $\omega = 1/\nu$[1, 10]; however, this result has recently been discussed by R.M. Ziff[11], who found instead $\omega = 1 + 1/\nu = 7/4$. We have performed a fit of $p_c(L)$ according to the above equation, leaving the exponent $\omega$ as a free parameter. The resulting $p_c(L = \infty)$ values are displayed in the last column of Table I and are determined with a good accuracy. In all cases, the value of the exponent $\omega$ is, within the error bars, more compatible with 0.75 than with 1.75, but the precision is too poor for a firm discrimination.

The extrapolated percolation threshold $p_c$, plotted in figure 1 as a function of $k$, first decreases rapidly, then flattens out and finally begins to
increase slowly for $k \geq 10$. This effect has previously been mentioned in ref. [5] and has been observed in a system of correlated site percolation [3]. We shall justify this rather unexpected behaviour by a change of the geometry of the configurations due to excluded volume effects.

This effect is visible in figure 2 which shows the percolating cluster at $p_c(L)$ for $k = 8$ (upper figure) and for $k = 32$ (lower figure) on the same lattice of size $L = 512$: for large $k$ ($k = 32$), the percolation cluster exhibits dense areas of aligned segments connected by low density regions, whereas the $k = 8$ cluster is much more uniformly distributed. In order to establish this effect more quantitatively, let us define the degree of alignment of the configuration in the following way: cover a given percolating configuration with a set of square boxes of size $\ell$; let $n_H$ be the number of sites covered by horizontal segments in a given box and $n_V$ the number of sites covered by vertical segments in the same box; the degree of alignment is given by

$$A(\ell) = \left\langle \frac{|n_H - n_V|}{n_H + n_V} \right\rangle$$

where the average is taken over the boxes which cover the configuration and over a sample of different configurations. Plotted in figure 3 as a function of $\ell$ for different values of $k$, this quantity slowly decreases down to 70% for box sizes $\ell \approx k$ and then falls rapidly like $1/\ell$ (dashed line) as expected from elementary statistics for a disordered system. This behaviour confirms the existence of regions of same orientation and whose typical size is the segment length $k$.

Assuming that the percolating cluster is an aggregate of such regions, the following argument explains qualitatively the behaviour of the percolation
threshold as a function of $k$. Let us assimilate a typical region of oriented segments to a rigid square box of size $2k$ and consider in it, a percolating cluster of $n$ segments ($n \leq 2k$). This cluster includes at least one segment originating at the bottom line of the box and at least one segment ending at the top line. The $n-2$ remaining segments ensure the connectivity, but their origins are randomly distributed among the $k$ allowed sites, giving to this cluster a statistical weight proportionnal to $k^{n-2}$. Its density is $nk/(2k)^2$, and decreases like $1/k$ as long as $n \ll 2k$, and is constant for $n \sim k$. Therefore, as $k$ increases, the relative weight of the dense clusters grows rapidly, and eventually the configurations are dominated by those clusters whose density remains constant with $k$. Assuming that the variations of the percolation threshold are driven by such a mechanism, one expects a $1/k$ decrease in the small $k$ regime, corresponding to the suppression of the light clusters, ending with a constant behaviour when the configurations become dominated by denser clusters. We have fitted our data according to this behaviour (continuous line in figure 1), and the agreement is quite good in the small $k$ regime. However, this modelisation of the oriented region by rigid boxes is presumably too simple to explain the slight rise for large $k$, which may be due to the interpenetrability of these regions and/or to their anisotropy.

This argument explains the change of geometry of the configurations observed in figure 2 - rather diffuse for small $k$ and denser for larger $k$ - as well as the stopping of the $1/k$ decrease of the percolation threshold as the segment length grows.

\[1\] A pure $1/k$ decrease has been observed in ref. 5 and explained by similar arguments
3 Non-universal exponent

The geometry of the percolative clusters is described by several fractal exponents, one of which is the fractal dimension of the infinite cluster $D$, which is linked to the percolation critical exponent ratio $\beta/\nu$

$$D = d - \frac{\beta}{\nu}$$

where $d$ is the space dimensionality. If finite range correlated site percolation is described by the random site percolation critical point, one expects for this fractal dimension the exact known value $D = 91/48$ \[1\]. However, the results of the previous section suggest that, as the segment length $k$ grows, the fractal dimension of the critical cluster doesn’t remain constant, but increases instead. Since $91/48$ is close to 2, in order to detect such a tiny effect one needs a very accurate determination of $D$.

Let $P(k, L, p)$ be the average size of the largest cluster on a lattice of linear size $L$, for segments of length $k$ and at a concentration $p$. According to finite size scaling, one expects:

$$P(k, L, p) = L^{2-\beta/\nu} F \left( \frac{k}{L}, \frac{L}{\xi} \right) = L^{2-\beta/\nu} F \left( \frac{k}{L}, L(p_c - p)^{\nu} \right)$$

(1)

where $\xi \simeq (p_c - p)^{-\nu}$ is the correlation length of the connected regions. The dependence on $k/L$ has been introduced to take into account the different length scales of the system, but since $k \ll L$, only the limiting value $F(0, y)$ is of interest, which we assume to be non-zero. According to this equation, one expects that at $p = p_c(L) = p_c - AL^{-1/\nu}$, the function

$$P(k, L, p_c(L)) \times L^{-2+\beta/\nu}$$

(2)

depends only on the ratio $k/L$ and tends to a non zero constant value as $k/L \to 0$. 

6
Alternatively, if there is not universality, the critical exponents become \( k \)-dependent and one expects

\[
P(k, L, p_c(L)) = L^{2 - \omega(k)} G(k/L)
\]

where \( \omega \) progressively deviates from \( \beta / \nu = 5/48 \) as \( k \) increases.

We have measured \( P(k, L, p_c(L)) \) for several values of \( k \) as a function of \( L \) in order to discriminate between these two different behaviour. This measure requires a very accurate determination of \( p_c(L) \), because \( P \) varies quite rapidly in this \( p \) region, from the non-percolating regime where the exponent is zero, to the percolating one, where the exponent is 2. We selected three values, \( k = 2, 8, 16 \), and determined \( p_c(L) \) with a precision less than 0.2% . Then we proceeded to the measure of \( P(k, L; p_c(L)) \). In order to take into account the systematic error induced by a small variation of \( p \), we have performed two measures, at \( p_c(L) \pm \Delta p_c(L) \), and the error bars displayed in the following figures represent the difference between the two results (the statistical errors are smaller than this systematic one).

In figure 4, we have plotted the quantity \( P(k, L, p_c(L)) \times L^{-91/48} \) as a function of \( k/L \), for the three \( k \) values. According to eq. 2 one should expect all the points to lie on the same universal curve. In spite of the rather large error bars, we see that this is not the case. In figure 5 we display \( P(k, L, p_c(L))/L^2 \) as a function of \( L \) in a Log-Log plot. The straight lines correspond to the best fit according to the power law of eq. 3 and with the exponents : \( \omega(k = 2) = 0.120 \pm 0.009 \), \( \omega(k = 8) = 0.084 \pm 0.011 \) and \( \omega(k = 16) = 0.011^{+0.020}_{-0.011} \). As \( k \) increases, one clearly observes a variation of the exponent \( \omega(k) \), away from the universal value \( \omega(k = 1) = 0.104 \).

All these results are more compatible with eq. 3 than eq. 2 and strongly
suggest that these systems are not in the random site percolation universality class.

4 Conclusion

In conclusion, we have exhibited a non-monotonic behaviour of the critical concentration for percolating systems of line segments deposited on a square lattice, as the segment length increases. We give a simple argument, based on the local alignment effect, which explains the change of structure of the critical clusters and the non-decreasing behaviour of the percolation threshold for large $k$.

The observed slow increase may have its origin in the effect proposed by Sanders and Evans [3] to explain similar behaviour in a correlated site percolation model based on an island forming process. In the limit of infinitely attractive force, this process favours the formation of large isotropic islands and evolves towards the continuous percolation model of Pike and Seager [7], with a threshold of 0.68, higher than for finite attractive force. Therefore, as the force strength increases the percolation threshold is pulled up toward this asymptotic value. It is tempting to establish a parallel between this model and our system in the following (speculative) way: the oriented regions of growing size play the role of the islands of the above-mentioned process, and eventually simulate a continuous percolation model for extended anisotropic objects. Assuming the same critical concentration $p_c \simeq 0.68$ as for the isotropic objects of Pike and Seager, we expect $p_c$ to increase toward this asymptotic value as $k$ increases. It is worth noticing that in this limit, the saturation coverage of the system is 0.66 [12] and the percolation con-
centration may well be unreachable.

Another consequence of the geometrical change of the configurations when $k$ varies, is that the various fractal exponents of the infinite cluster may depend on $k$. Our results strongly suggest that the fractal dimension of the infinite cluster, linked to the ratio of the critical exponents $\beta$ and $\nu$, slowly increases, thus indicating for these systems a departure from the expected random site percolation universal behaviour.

However, this effect appears as a small signal, and in spite of a careful analysis one cannot rule out the possibility of systematic errors due, for instance, to some underestimated finite size effect linked to a too small $L/k$ ratio. Therefore these results need to be confirmed by a determination of other critical exponents linked to the cluster structure, such as $\gamma$, which is characteristic of the average cluster size. Furthermore, if a violation of universality is definitely established, one must explain its origin. Presumably, the anisotropy of the percolating objects plays a role, and, for large segments, the transition may induce a large scale anisotropy. In this case, one should characterise the scaling properties of the percolating clusters by critical exponents in both lattice directions, just like in the directed percolation model [13]. These various aspects of the model are currently under investigation.

Acknowledgements
We thank F. Carmona for several helpful discussions and J.T. Donohue for a careful critical reading of the manuscript. YL thanks Jim Evans for pointing out ref. [3] to him.
References

[1] *Introduction to percolation theory*, D. Stauffer, (Taylor and Francis, London, 1985)

[2] *Percolation structures and processes*, Ann. Isr. Phys. Soc. Vol. 5, edited by G. Deutsher, R. Zallen and J. Adler, 1983.

[3] Sanders D.E., Evans J.W. *Phys. Rev. A*38, 4186 (1988)

[4] M. Nakamura, *Phys. Rev.* A36, 2384 (1987)

[5] Carmona F., Barreau F., Delhaes P. and Canet R. *J. Physique Lett.* 41, L534 (1980)

[6] Boissonade J., Barreau F., Carmona F. *J. Phys. A*16, 2777 (1983)

[7] G.E. Pike and C.H. Seager, *Phys. Rev. B*10, 1421 (1974)

[8] I. Balberg, N. Binenbaum *Phys. Rev. B*28, 3799 (1983)

[9] Experiment in progress at LCPC, Bordeaux University, J.P. Aime private communication.

[10] P.J. Reynolds, H.E. Stanley and W. Klein, *J. Phys. A*11,L199 (1978)

P.J. Reynolds, H.E. Stanley and W. Klein, *Phys. Rev. B*21, 1223 (1980)

[11] R.M. Ziff, *Phys. Rev. Lett.* 69, 2670 (1992)

[12] B. Bonnier, M. Hontebeyrie, Y. Leroyer, C. Meyers and E. Pommiers, to appear in *Phys. Rev. E*

[13] for a review, see the article of W. Kinzel in ref. [2]
Table I: The percolation threshold for various segment lengths $k$ and lattice sizes $L$. The last column corresponds to the extrapolated value. Numbers in parentheses are the errors affecting the corresponding final digits.

| $k$ \ $L$ | 128   | 256   | 384   | 512   | 680   | 850   | 1024  | $\infty$ |
|-----------|-------|-------|-------|-------|-------|-------|-------|---------|
| 1         | 0.586(5) | 0.589(6) | 0.590(7) | 0.590(9) | 0.590(4) |       |       | 0.593(1) |
| 2         | 0.555(4) | 0.557(4) | 0.558(3) | 0.559(2) |       |       |       | 0.561(1) |
| 4         | 0.498(2) | 0.500(9) |       |       |       |       |       | 0.504(3) |
| 8         | 0.456(8) | 0.462(8) | 0.465(6) | 0.465(4) |       |       | 0.467(5) | 0.470(1) |
| 16        | 0.442(1) | 0.450(7) | 0.456(8) | 0.457(7) | 0.459(1) | 0.460(1) | 0.461(1) | 0.463(1) |
| 24        | 0.445(3) | 0.458(2) | 0.459(2) | 0.462(1) | 0.462(1) | 0.464(1) | 0.466(1) |         |
| 32        | 0.402(3) | 0.450(2) | 0.462(3) | 0.466(1) | 0.467(2) | 0.467(1) | 0.469(1) | 0.471(1) |
| 40        | 0.450(2) | 0.461(1) | 0.467(1) | 0.470(2) | 0.474(2) | 0.475(2) | 0.484(6) |         |
Figure captions

Figure 1 The extrapolated percolation threshold as a function of the segment length $k$. The continuous line is a fit in $1/k + \text{const}$.

Figure 2 Two percolating clusters, for segments of length $k = 8$ and $k = 32$, on a lattice of size $L = 512$.

Figure 3 The degree of alignment (as defined in the text) as a function of the block size $\ell$, for different segment lengths. The dashed lines are fits in $1/\ell$ of the tails of the distributions.

Figure 4 The quantity $P(k, L, p_c(L)) \times L^{-91/48}$ as a function of $L/k$ for three values of the segment length $k$.

Figure 5 The quantity $P(k, L, p_c(L))/L^2$ as a function of $L$ for three values of the segment length $k$. The dashed straight lines are the power law fits.