Geometry of fully coordinated, two-dimensional percolation

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We study the geometry of the critical clusters in fully coordinated percolation on the square lattice. By Monte Carlo simulations (static exponents) and normal mode analysis (dynamic exponents), we find that this problem is in the same universality class with ordinary percolation statically but not so dynamically. We show that there are large differences in the number and distribution of the interior sites between the two problems which may account for the different dynamic nature.

05.40.Fh, 05.70.Fh, 05.70.Jk, 64.60.Ak, 68.35.Rh

I. INTRODUCTION

The geometrical phase transition known as percolation (see, for a review, Stauffer and Aharony [1]) is appreciated by many to be an elegant and simply defined yet fully featured example of a second order phase transition. A number of variations of the original percolation problem were proposed as better models of some physical phenomena in the past. This includes the backbone percolation for studying electrical conduction through random media, polychromatic percolation for multi-component composites, and four-coordinated bond percolation for hydrogen-bonded water molecules. In particular, Blumberg et al [3] and Gonzalez and Reynolds [4] studied a random bond, site-correlated percolation problem they call four-coordinated percolation on the square lattice. They conclude that this problem belongs to the same universality class as the ordinary random percolation with the same set of (static) exponents.

In this paper, we revisit a problem in this realm, though not exactly the same one. We define fully coordinated percolation as the site percolation problem where only the occupied sites all of whose neighboring sites are also occupied can transmit connectivity. Since the random element is the site, this problem is slightly different from the bond problem referred to above. Thus, after generating a random site configuration with the independent site occupation probability \( p \), we only select those occupied sites with all 4 neighbors also occupied on the square lattice and study the clusters formed by nearest neighbor connections among those sites. It should be noted that this problem is distinct from the so-called bootstrap percolation (see, e.g., [3]) where sites of less connectivity are iteratively removed. In our problem, no iterative procedures are involved; rather, sites of less than full connectivity are marked first and then all of them removed at one time.

This problem arose in the context of studying the vibrational properties of fractal structures tethered at their boundaries [5]. In that problem, scaling was observed in the normal mode spectrum whose origin may lie in the ratio of 2 length scales, one of which is the size of highly connected regions of a cluster. In this context, we have embarked on revisiting the characteristics of randomly generated, but highly connected geometrical structures.

In the next section, we summarize the Monte Carlo and finite size scaling analyses of the static critical properties of fully coordinated percolation. In Section 3, we discuss the normal modes of the transition probability matrix for tracer diffusion on the structure using the methods of Arnoldi and Saad (see, e.g., [6]). Then in Section 4, we describe the classification of the cluster sites into external boundary, internal boundary, and interior ones and using these to show the major distinctions between the critical clusters of ordinary and fully coordinated percolation. We summarize the results in the final section.

II. STATIC CRITICAL BEHAVIOR

To determine the static critical behavior of fully coordinated percolation we first performed Monte Carlo simulations on a square lattice in two dimensions. Each site is occupied with probability \( p \) independently and subsequent fully coordinated sites are marked and their connectivity searched. Lattice sizes of \( L^2 \) where \( L = 256, 512, 1024, \) and 2048 were constructed. For each lattice size we further made a thousand realizations wherein a different random number seed was used on every run.

The unnormalized susceptibilities, i.e., \( \Xi(L) = \sum_s s^2 \hat{n}_s \) where \( \hat{n}_s \) is the number of clusters of size \( s \), are calculated on each run and are then summed at the end of the thousand realizations. The average susceptibilities \( \chi \) are calculated by dividing the sum by the number of realizations and the lattice size. The prime on the summation indicates the fact that the contribution of the largest cluster to \( \chi \) is near and above what we perceived to be the critical probability \( p_c \) has been subtracted as usual [4].

In Fig. 1 we plot the average susceptibilities against the probability \( p \) for the corresponding lattice sizes. The data correspond to the values of \( L = 256, 512, 1024, \) and 2048 from the lowest to highest. We can see that the effects due to the finite sizes of the lattices are exhibited clearly. In particular, there are well-defined peaks which
scale with lattice sizes as
\[
\chi(p_{\text{max}}, L) \sim L^{\gamma/\nu}
\]
where the known exact value of \(\gamma/\nu\) for the ordinary percolation is \(\frac{41}{42} \sim 1.7917\). To demonstrate the precision of our calculations, we plot \(\chi(p_{\text{max}}, L)\) against the corresponding lattice sizes in the inset of Fig. 1. Notice that the data follow an excellent power law, leading to a least squares fit of \(\chi(p_{\text{max}}, L) \sim L^{1.7911}\). The value of \(\gamma\) found is identical with the ordinary percolation value to within about 0.03%. This result confirms previous work [3,4] stating that fully coordinated percolation and ordinary percolation belong to the same static universality class.

The critical behavior of susceptibility is known to scale as

\[
\chi(p, \infty) \sim |p - p_c|^{-\gamma}
\]
where for ordinary percolation \(\gamma_o = \frac{41}{42} \sim 2.3889\). Notice however that in Fig. 1 the peaks are very near \(p = 1.0\). This would provide data to the right of the peaks in only a small probability interval. In our simulations, we would therefore use \(\gamma\) only to the left of the peaks.

Since the scaling relation in Eq. (1) is expected only for infinite lattices, we use only the data taken from \(L = 2048\) to test it. Since there are two unknowns in Eq. (1), we first choose a particular \(p_c\) and make a fit to see what value of \(\gamma_{\text{exp}}\) is obtained. If we choose \(p_c = 0.886\) we get \(\gamma_{\text{exp}} = 2.4004\). The correlation coefficient, \(|R|\), for this fit is 0.99999. The discrepancy between \(\gamma_{\text{exp}}\) and \(\gamma_o\) is around 0.481%. Choosing \(p_c = 0.8858\) we obtain \(\gamma_{\text{exp}} = 2.3864\). The discrepancy this time is around 0.10% and \(|R| = 1.0\). So we have an exact fit for this value of \(p_c\) and the \(\gamma_{\text{exp}}\) found is very close to the \(\gamma_o\). Choosing \(p_c = 0.885\) we obtain \(\gamma_{\text{exp}} = 2.3302\) with an \(|R| = 0.99999\). The discrepancy for this value of \(p_c\) is 2.46%. Fits done with \(p_c\) between 0.885 and 0.886 gave \(|R| = 1.0\); however, the \(\gamma_{\text{exp}}\) found when \(p_c = 0.8858\) gave the closest value to \(\gamma_o\). This allows us to conclude that \(\gamma\) for fully coordinated percolation is the same as that for ordinary percolation while also giving an estimate for the value of \(p_c\) close to 0.8858. (We will state the experimental uncertainty for \(p_c\) after all our analyses are presented.)

From the fit done to examine the scaling in Eq. (1) we could further conclude that \(\nu\) for fully coordinated percolation should be the same with that for ordinary percolation. This again confirms the statement that fully coordinated percolation is in the same static universality class as ordinary percolation. Another universal constant often used to characterize ordinary percolation is the amplitude ratio \(C_+/C_-\) of susceptibility \(\chi\) (whose value is about 200 in \(d = 2\) [3]). In fully coordinated percolation, this quantity is unfortunately difficult to calculate accurately because the critical region for \(p > p_c\) is very small (see below). When we constrain the exponent \(\gamma\) to be close to \(\gamma_o\) and use the \(p_c\) estimated in this work, however, we find that \(C_+/C_-\) is of \(O(10^2)\), which is consistent with the above observation as well.

The contribution of the largest cluster to the susceptibility is not significant when \(p < p_c\). However when \(p \sim p_c\) a significant number of sites will belong to the largest cluster and when \(p > p_c\) the largest cluster is dominant in the whole lattice. The average susceptibility contribution due to this largest cluster is \(\chi_1 = \sum s_{\text{max}}^2/(L^2N)\), where the summation is over \(N = 1000\) realizations and \(s_{\text{max}}\) is the size of the largest cluster. The fractal dimension, \(d_f\), can be obtained from \(s_{\text{max}}\) by

\[
s_{\text{max}}(p_c) \sim L^{d_f}
\]

where \(\pi_{\text{max}}(p_c)\) is the mean size of the largest cluster at \(p_c\). \(\chi_1\) should therefore scale as

\[
\chi_1 \sim L^{2d_f - 2}.
\]

For ordinary percolation on a two dimensional lattice (see, e.g., [2]), it is known that \(d_f = 91/48\) and \(y \equiv 2d_f - 2 \sim 1.7917\). For fully coordinated percolation, the scaling in Eq. (1) has two unknowns, \(p_c\) and \(d_f\). Similar to what we have done when examining the scaling in Eq. (1), we choose trial values for \(p_c\) and then perform a least squares fit to obtain the corresponding \(y = 2d_f - 2\). By looking for the range of trial \(p_c\) that maximizes the regression coefficient \(|R|\), we arrive at an estimate of \(p_c\) to be close to 0.8845 where \(|R| = 1\) and \(y = 1.7855\). The variation of \(|R|\) is about 2 parts in \(10^5\) if \(p_c\) is varied by 0.0002, always with less than 1% deviation from the ordinary percolation value of \(y\). From these results we conclude that \(d_f\) for fully coordinated percolation is the same as that for ordinary percolation as well as the estimate of about 0.8845 for \(p_c\).

In addition to the above, we have also performed the scaling analysis of the quantity \(\chi_1(p, L)\), as both \(p\) and \(L\) are varied, in the form of

\[
\chi_1 = L^{2d_f - 2} g(|p - p_c|^{\nu} L)
\]

where \(g(|p - p_c|^{\nu} L)\) is a scaling function. Using the exactly known ordinary percolation values of the exponents \(d_f\) and \(\nu\) (as they have been shown to be the same for fully coordinated percolation above), we obtained the maximum data collapsing in the range of 0.884 < \(p_c\) < 0.885.

Independent of the above analyses based on the fully coordinated clusters obtained by Monte Carlo simulations of fixed-sized square grids, we have also performed Monte Carlo simulations by growing fully coordinated clusters starting from a seed site using a variant of the breadth-first search algorithm [3]. This latter approach has an advantage that there is no obvious finite-size effects and that statistics taken while a cluster is still growing represents a partial sum automatically. That is, we start growing such clusters 10,000 times at each of \(p = 0.880, 0.884, 0.885, \text{ and } 0.890\), and keep track of how many of them are still growing at predetermined intervals of size \(2^n\) where \(n = 1, 2, \ldots, 15\) in our case). This number, say, \(N_s\) represents the partial sum
\[
N_s/N_1 = \frac{1}{p} \sum_{s' \geq s} s' n_{s'}
\]  

(6)

Since the normalized number of size-\(s\) clusters, \(n_s\), scales as \(s^{-\tau} f(\epsilon s^\sigma)\) where \(\tau = 187/91\) and \(\sigma = 36/91\), we expect that \(N_s\) scales as

\[
N_s s^{s-2} \sim \tilde{f}(\epsilon s^\sigma)
\]

(7)

near \(p_c\) and for large \(s\). In particular, at \(p_c\), this quantity should be constant independent of (large) \(s\). The numerical results are shown in Fig. 2, where the data correspond, from highest to lowest, to \(p = 0.890, 0.885, 0.884,\) and 0.880. The horizontal dashed line drawn to guide the eye makes it clear that data for \(p = 0.885\) best approximates a horizontal line as \(s \to \infty\), suggesting that a good estimate of \(p_c\) would be 0.885.

We now consider all the above results together. The results from scaling in Eq. (3) indicate a range 0.885–0.886, and those from scaling in Eq. (4) indicate 0.884–0.8847, while those from scaling in Eq. (5) hints \(p_c\) to be in the 0.884–0.885 interval. Another result that could also be used are the values of \(p\) for the peaks in Fig. 1, which vary from 0.8841 to 0.8844 (with the peak for the largest grid \(L = 2048\) occurring at \(p_{\text{peak}} = 0.8844\)). Combining all these results, our final estimate is \(p_c = 0.885 \pm 0.001\).

III. DYNAMIC CRITICAL BEHAVIOR

By dynamic critical behavior here we simply mean the asymptotic long-time behavior of diffusion taking place on an incipient infinite cluster of fully coordinated percolation, or its equivalent scalar elastic behavior. This represents the simplest kind of dynamics associated with these complicated geometrical objects and is mainly reflected in the two dynamic critical exponents called \(d_s\) (spectral dimension) and \(d_w\) (walk dimension).

It is well known that the return-to-the-starting point probability of the random walk, \(P(t)\), in the long-time limit obeys the power law,

\[
P(t) \sim t^{-d_s/2},
\]

(8)

where \(d_s\) is the spectral dimension of the walk. In a fractal medium, \(d_s\) is less than the space dimension \(d\), because the progressive displacement of the random walker further from the starting point is hampered by its encounter with the irregularities of the medium at all scales. Thus, \(d_s\) is expected to be greater for environments that provide higher connectivity at large length scales, independently of the fractal dimension itself which is mainly the measure of the overall size scales or how many sites are connected, not how well those sites are connected to each other.

For media with long-range loops, \(d_f\) (fractal dimension), \(d_s\), and \(d_w\) are not independent but are expected to obey the well-known Alexander and Orbach scaling law [10].

\[
d_s = 2d_f/d_w.
\]

(9)

For this reason, we only calculate \(d_s\) here though both of \(d_s\) and \(d_w\) can be conveniently calculated by numerically studying the transition probability matrix \(W\) which represent the random walk on a specific fractal medium. Our calculation in this work is only one aspect of such an analysis: finite size scaling of the dominant non-trivial eigenvalue which describes the longest finite time scale of the Brownian process. This approach has already been described in detail elsewhere [11], and thus we merely state the main feature and then immediately report our specific numerical results.

The matrix \(W\) is constructed from the elements \(W_{ij}\) being equal to a hopping probability per step (equal to \(\frac{1}{4}\) here) for available nearest neighbor sites \(i\) and \(j\). For each neighbor site which is not present, a probability of \(\frac{1}{4}\) is added to the probability for not taking a step for one time period - this is called the blind ant rule. Many large matrices \(W\) are obtained by Monte Carlo simulation (by growing a fully coordinated percolation cluster from a seed site and stopping the growth when a pre-determined desired size is reached) and their largest eigenvalues are numerically obtained by the so-called Arnoldi-Saad method. The dominant non-trivial eigenvalue \(\lambda_1\) is the largest eigenvalue just below the stationary eigenvalue 1 and it is known to satisfy the following finite size scaling law:

\[
|\ln \lambda_1| \approx 1 - \lambda_1 \sim S^{-2/d_s}.
\]

(10)

Shown in Fig. 3 are our results from such an analysis. We have generated at least 1000 independent realizations of the underlying fully coordinated percolation clusters for sizes \(S = 1250, 2500, 5000, 10000,\) and 20000 at each of the three nominal probabilities \(p = 0.883, 0.885,\) and 0.887, and numerically obtained \(\lambda_1\) for each cluster. The main part of Fig. 3 shows the data from \(p = 0.885\), the value shown to be closest to \(p_c\) in this work. The figure shows an excellent power law fit (regression coefficient of -0.99993) to Eq. (10) with the exponent 2/\(d_s\) = 1.486 ± 0.01. This power translates to \(d_s = 1.346 \pm 0.011\) which is close to but definitely larger than the corresponding ordinary percolation value of \(d_s^{(O)} = 1.30 \pm 0.02\) estimated by many independent calculations. (See, e.g., [12].) For comparison, a loopless variant of percolation has exactly the same static exponents as ordinary percolation but has \(d_s = 1.22\) in two dimensions, about twice as much deviation from ordinary percolation in the opposite direction as the present fully coordinated percolation problem.

In the inset for Fig. 3, we show a normalized \(\lambda_1\) by plotting \((1 - \lambda_1)S^{2/d_s^{(O)}}\) where the circles are for \(p = 0.887\), squares for \(p = 0.885\), diamonds for \(p = 0.883\) and the solid line is a horizontal line (for ordinary percolation) to guide the eye. In all cases, the standard errors of the mean for each set of data are substantially smaller than the size of the symbols used in the figure. The
distribution of $\lambda_1$ in each case appears to be Gaussian with the standard deviations scaling in the same way as the means.

From these results, we conclude that, though the numerical differences are small, there is a high likelihood that the fully coordinated percolation clusters are significantly different from the ordinary percolation counterparts even at long length scales. In the next section, we show that this analysis is vindicated by exposing one dramatic difference in the cluster morphology which will not be obvious to an uncritical observer.

IV. CLUSTER GEOMETRY

In this section we examine the geometry of fully coordinated percolation clusters more closely. First, we present Fig. 4 which show in grey scale the sites of (a) fully coordinated percolation cluster and (b) ordinary percolation cluster at respective $p_c$. The overall visual impression is that they are very similarly shaped even down to the details of the boundaries and internal holes. Their shapes are also essentially independent of the underlying lattice anisotropy (as Fig. 4(a) has actually been rotated by 45 degrees with respect to the coordinate axes of the square lattice). However, the number and distributions of the especially dark points are evidently quite distinct in (a) and (b). They cluster more and are much more abundant in (a) than in (b). These sites are actually the interior or fully coordinated sites in the internal part of the cluster. The remaining sites (shaded grey) are either the external hull sites or internal boundary sites.

In Fig. 5 quantitative examination is made on the different classes of sites of the two kinds of clusters. In the main part of the figure, the average numbers of two kinds of sites are shown, interior (diamonds for fully coordinated percolation, crosses for ordinary percolation), and external (squares for fully coordinated percolation, plusses for ordinary percolation). It is clear that the interior sites are more than 3 times abundant in fully coordinated percolation as is visually suggested by Fig. 4. Though this is primarily a local effect due to the full coordination rule, they do have a multiplicative effect at long-range connectivity and thus may well be the source of the small difference in the value of $d_s$.

Of course just the fact that there are more than 3 times as many interior sites (and correspondingly, much fewer hull sites) in fully coordinated percolation must have quantitative consequences (even if not qualitative) for any process on the cluster which depend on degrees of connectivity rather than just on the number of connected sites. An example of the effect of the different numbers of the hull sites may be in oxidation or catalysis of a material through the external embedding phase or even a irregularly shaped breakwater in the form of the external boundary of a percolation cluster. The external sites are those which are sometimes called hull sites and they are known to scale with an exact exponent in ordinary percolation as

$$N_{\text{hull}} \sim S^{d_h/d_f}$$

where $d_h^{(o)} = 7/4$ and thus the exponent is $84/91 = 0.923...$ for ordinary percolation. Since this is less than 1, these sites comprise less and less fraction of the cluster as $s \to \infty$ and the remaining sites (i.e., interior and internal boundary sites) eventually dominate the whole cluster. This is already evident from the greater slopes close to 1 for the interior sites in Fig. 5. The linear regression fits for the hull sites in Fig. 5 indicate the slopes of about 0.913 for ordinary percolation and 0.922 for fully coordinated percolation with essentially perfect fits, again reinforcing the conclusion that they show the same static critical behavior.

V. SUMMARY AND CONCLUSION

In summary, we have studied both static and dynamic critical behaviors associated with a model of the highly connected regions of a disordered cluster. The model is a site variant of the four-coordinated percolation $\bullet \bullet \bullet$ on the square lattice we call fully coordinated percolation. While the bond version was studied for static critical behavior, neither bond nor site version was previously studied for the dynamic behavior to the best of our knowledge. We have used various methods such as Monte Carlo simulations, finite-size scaling and Arnoldi-Saad approximate diagonalization of large random matrices for this purpose.

Though all indications are that the static behavior of this model is exactly the same as the ordinary percolation (as previous work suggested), the dynamic behavior shows a small but significant difference in the values of the universal critical exponents. We have looked for the cause of this difference and found a three-fold increase in the number and significantly enhanced clustering of the interior sites (i.e., those not on the exterior or internal boundaries) and the associated decrease in the number of boundary sites. Thus, although the deviations from ordinary percolation in terms of the values of the dynamic critical exponents are not large, there will be rather significant differences in any processes that depend sensitively on those numbers. Possible examples of such processes include the oxidation of a material through the external embedding phase and the vibrational normal modes with boundary conditions such as clamping or tethering of the external boundaries (through the contrast in elastic constants of embedding and embedded materials, for example).
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FIG. 1. Susceptibilities $\chi$ for fully coordinated percolation on finite square lattices of size $L^2$ are shown against probability $p$, where crosses, diamonds, squares, and circles are for $L = 256, 512, 1024$, and 2048, respectively. The inset shows the finite-size scaling of the peaks of these curves by plotting the maximum $\chi$ vs. $L$ on a log-log scale.

FIG. 2. The scaled partial sum $N_s$ is plotted against $s^\sigma$ for $p = 0.890$ (cross), 0.885 (circle), 0.884 (triangle), and 0.880 (plus). The dashed line is a horizontal line to guide the eye, showing that the data for $p = 0.885$ best fits the horizontal slope for large cluster sizes. The inset shows a normalized $\lambda$ (see text) for $p = 0.887, 0.885, \text{and} 0.883$ (from top). The solid line is horizontal, corresponding to the slope for ordinary percolation.

FIG. 3. The scaling of the largest nontrivial eigenvalue $\lambda_1$ of the Markov chain analysis is shown by plotting $1 - \lambda_1$ against the cluster size $s$ on a log-log scale. The inset shows a normalized $\lambda$ (see text) for $p = 0.887, 0.885, \text{and} 0.883$ (from top). The solid line is horizontal, corresponding to the slope for ordinary percolation.

FIG. 4. (a) A typical fully coordinated percolation cluster at its $p_c$, and (b) the corresponding critical ordinary percolation cluster. The dark points are the interior sites of full coordination and the grey shaded sites are either on the external hull or internal boundaries.

FIG. 5. The numbers of external sites (squares and plusses) and those of interior sites (diamonds and crosses) are scaled against the cluster size $s$. The solid (fully coordinated percolation) and dashed (ordinary percolation) lines are the linear least squares fits. In the inset, we show the number of external sites divided by $s^{d^{(e)}_h}\sigma^{d^{(e)}_f}$, showing that the population of the external hull sites of fully coordinated and ordinary percolation scale in the same way.
\[ \chi(L) = \Sigma' \cdot s^2 \cdot n_s \]

Fig. 1  (Cuansing, Kim & Nakanishi)
Fig. 3  (Cuansing, Kim & Nakanishi)
