

Site percolation on lattices with low average coordination numbers

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Abstract. We present a study of site and bond percolation on periodic lattices with (on average) fewer than three nearest neighbors per site. We have studied this issue in two contexts: by simulating oxides with a mixture of 2-coordinated and higher-coordinated sites and by mapping site-bond percolation results onto a site model with mixed coordination number. Our results show that a conjectured power-law relationship between coordination number and site percolation threshold holds approximately if the coordination number is defined as the average number of connections available between high-coordinated sites and suggest that the conjectured power-law relationship reflects a real phenomenon requiring further study. The solution may be to modify the power-law relationship to be an implicit formula for percolation threshold, one that takes into account aspects of the lattice beyond spatial dimension and average coordination number.

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1. Introduction

Percolation is a simple phase transition that can occur in a great many systems that exhibit branched network structure [1, 2]. The basic idea is that one occupies, at random, either the components of the system (often sites on a lattice) or the links between the components (bonds between sites). As the occupation probability per site (or bond) increases, clusters of connected elements form and grow. When the occupation probability exceeds a critical value p_c , there is a cluster that spans the length of the system (or wraps, in simulations with convenient periodic boundary conditions), from one side to the other. In the context of a lattice, one could envision the percolating cluster as being a continuous object that touches both sides of the system. Percolation theory has applications in a great many contexts, ranging from materials science topics such as gelation or transport in porous media, to societally relevant contexts such as disease propagation and forest fires.

The percolation threshold is only known exactly for special classes of lattices, all in 2D [3, 4]. For most systems one must use Monte Carlo simulations to compute p_c [5]. One determines p_c in simulations by occupying sites (or bonds) one-at-a-time in a random order, stopping when the occupation of one more site (or bond) results in the formation of a wrapping cluster. Different random orders give percolation at different

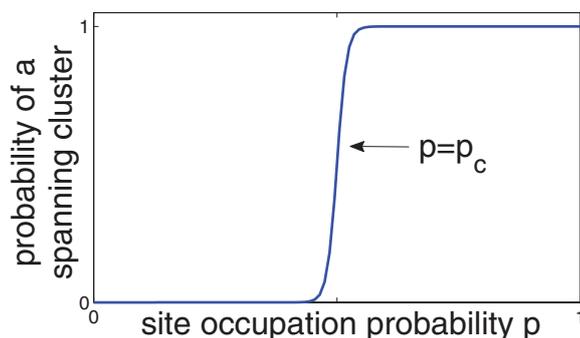


Figure 1. Example plot of percolation probability versus site occupation probability.

site occupation fractions and after a large number of lattices have been simulated one obtains a sigmoidal plot of percolation probability (i.e. probability of a wrapping cluster forming) versus site occupation probability (figure 1). The percolation threshold is the point on the plot at which the wrapping probability rises rapidly from zero to one.

Despite the paucity of exact results, analytical formulas have been proposed to provide approximate predictions (of varying accuracy) for p_c on different lattices, e.g. [6–12]. One physically intuitive approximation for the percolation threshold is a power-law relation, noted by Galam and Mauger, between coordination number z and percolation threshold p_c [7]. Power-law behavior is ubiquitous in critical phenomena and the power-law relation is known to give reasonably accurate predictions of p_c for many lattices with $z \geq 4$ in 2, 3 and sometimes higher dimensions. This power-law relation has found application to a number of problems in physics [13, 14] and even social science [15]. Recently, it has also been shown to give fairly accurate predictions of p_c for z as low as 3 in 3D [16].

The power-law relation has been shown to be problematic in regards to its predictive power and accuracy [10], [17–20]. For instance, lattices are grouped by Galam and Mauger into three different universality classes, but the theory provides no criterion for determining which class a lattice should belong to. Moreover, there are many situations in which two lattices have the same coordination number and dimensionality, but due to differences in higher-order aspects of structure their percolation thresholds differ, e.g. the triangular and octagonal lattices in 2D (which have the same site percolation threshold but different bond percolation thresholds) [18], or the body-centered cubic and stacked triangular lattices in 3D [17]. The power-law scaling formula also lacks a number of other properties that would be desirable in any accurate and widely-applicable predictor of percolation thresholds [10]. Despite these problems, the power-law formula of Galam and Mauger remains of some interest because it shows a common (if not universal) trend of approximately power-law behavior in a phase transition.

It is natural to ask whether this power-law scaling of p_c continues to hold for $z < 3$. While it is impossible to construct an interesting lattice in which *all* of the sites have $z < 3$ (it would just be a linear chain), one can still construct very interesting lattices in which *some* of the sites³ have $z = 2$ and others have $z \geq 3$. The $z = 2$ sites can make

³ One could also consider a lattice in which some sites have $z = 1$, i.e. some dangling atoms, analogous to the role of singly-bonded hydrogen in a macromolecule, but from a percolation standpoint such lattices are uninteresting. The occupation of a $z = 1$ site cannot connect two clusters to form a single cluster that wraps around the system and thus it can be eliminated from the model without affecting any conclusions concerning connectivity and transport.

the lattice analogous to some oxides, with 2-coordinated sites (analogous to oxygen atoms) joining together exactly two other sites.

Unfortunately, the conjectured power-law relation cannot remain valid when the average coordination number gets sufficiently close to 2. The power-law formula is:

$$p_c = p_0((d-1)(z-1))^{-a} \quad (1)$$

where $a = 0.6160$ and $p_0 = 1.2868$ for site percolation on 2D kagomé lattices and regular lattices in 3 or more dimensions and $a = 0.3601$ and $p_0 = 0.8889$ for simple 2D lattices (e.g. square, honeycomb and triangular). For $z = 2$ and $d = 3$ it predicts $p_c < 1$, when it should obviously be 1 for $z = 2$ (which corresponds to a 1D chain). Given that this relationship cannot remain valid for z arbitrarily close to 2, but that it does work (to within 4%) for $z = 3$ [16], it is reasonable to explore other low- z cases to determine the accuracy of the power-law scaling relation.

The introduction of 2-coordinated sites along the bonds of a lattice is equivalent to introducing a mixed site-bond problem, in which sites are occupied with probability p_s and bonds are occupied with probability p_b [21]. If we place a single oxygen atom (2-coordinated site) along each bond and treat the 2-coordinated sites the same as the other sites (i.e. occupy them with the same probability as other sites), we have a site-bond problem with $p_b = p_s$. Physically, one could visualize this problem as corresponding to an oxide, in which the two-coordinated sites correspond to oxygen atoms and the higher-coordinated sites correspond to atoms of higher valence. Alternately, if one wished to visualize these problems in terms of communications networks or similar phenomena, the 2-coordinated sites would correspond to possible points of failure in connections between network nodes. If we introduce additional 2-coordinated sites (i.e. more than one per bond) and continue to treat them on an even footing with the other sites we have a problem with $p_b < p_s$. This equivalence between a problem with low coordination number and a site-bond percolation problem enables us to use existing results for site-bond percolation to probe site percolation on lattices with $z < 3$.

However, setting up a lattice with average coordination number less than 3 and finding its percolation threshold is not sufficient for understanding the behavior of p_c at low z . We also need a proper quantitative measure of average coordination number on that lattice. There are a number of plausible approaches that one could take. Intuitively, one could compute the average number of neighbors per site, an approach based on the structure of the lattice. Alternately, one could compute the average number of available bonds between high-coordinated sites, an approach based on the connectivity of the lattice at a particular occupation fraction and one that we will show to be useful in this work.

To illustrate the difference between these measures, consider the lattice in figure 2. It is a square oxide structure, with a 3-atom basis outlined in red. The average coordination number per site is easy to compute. There are two atoms with two neighbors apiece and there is one atom with four neighbors. The average coordination number is thus $\bar{z} = (1 \cdot 4 + 2 \cdot 2) / 3 \approx 2.667$. However, forming a cluster that wraps around the system requires linking 4-coordinated sites to one another. If we occupy sites with probability p and treat the 4-coordinated sites on the same basis as 2-coordinated sites (i.e. occupy each type of site with the same probability) then the average number of

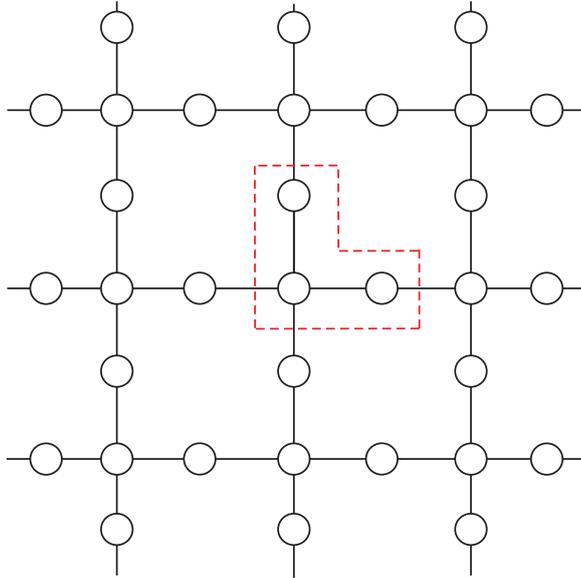


Figure 2. A simple example of a lattice with low average coordination number. The underlying Bravais lattice is square and the basis (outlined in red) is three atoms (one 4-coordinated, the others 2-coordinated).

sites occupied between the 4-coordinated sites is $4p$ and thus each 4-coordinated site has connections to (on average) $4p$ other sites (which may or may not be occupied). More generally, if we start with a lattice on which each site has coordination number $z_1 \geq 3$, introduce (possibly multiple) 2-coordinated sites along some or all of the bonds and occupy those sites in such a way that there is a probability p_b of having an unbroken bond between the z_1 -coordinated sites, the average number of accessible neighbors per z_1 -coordinated site will be $p_b z_1$. We will show here that choosing the later measure (number of bonds between high-coordinated sites) leads to a more robust scaling between percolation threshold and coordination number for lattices with mixed coordination numbers.

In what follows we will study lattices with low coordination number in two different ways: First, we will use Monte Carlo simulations to compute site percolation thresholds on three oxide-type lattices with average coordination number less than 3: the SiO_2 lattice (a diamond lattice with 2-coordinated oxygen atoms along the bonds) and two 3-coordinated lattices ((10,3)-a and (10,3)-b [16, 22]) with 2-coordinated oxygen atoms introduced along their bonds. As a check on the scaling behavior of p_c at low coordination number we will also study a ‘cubic oxide’ with average coordination number 3. We will show that the percolation thresholds of these lattices are consistent (to better than 2% and in two cases to better than 0.1%) with the power law conjectured by Galam and Mauger if average coordination number is defined in terms of the average number of bonds between high-coordinated sites rather than the average number of neighbors per site. Second, using existing data on site-bond percolation problems [21], we will map mixed site-bond problems onto pure site percolation problems with low coordination numbers and show that power-law scaling of p_c with z again holds if the average coordination number is measured by the average number of bonds per high-coordinated site. Based on these results, we conjecture that power-law scaling between

p_c and z holds if one defines z in terms of available links between higher-coordinated sites, leading to an implicit formula for p_c that incorporates aspects of lattice structure beyond dimensionality and average coordination number.

2. The oxide lattices studied

We begin by briefly describing the four lattices that we are studying here: silicon dioxide, (10,3)-a oxide, (10,3)-b oxide and cubic oxide. We will describe the structure of these lattices in their most symmetric forms, so that the reader can visualize them in plausible physical realizations. However, as in our previous work [16], for computational purposes we deformed the bond orientations so that the lattices could be mapped onto cubic grids, albeit with fewer than six bonds to each site. Percolation thresholds are governed only by the presence of the bonds, not their orientations. Deforming the lattice in a way that preserves the connections between sites does not change its percolation threshold, but leads to greater convenience in enumerating sites. The process of this deformation for (10,3)-a and (10,3)-b can be seen in greater detail in our previous work.

2.1. Silicon dioxide

The silicon dioxide lattice is based on the diamond lattice, which is a face centered cubic lattice whose primitive cell consists of two lattice points. Each site is connected to four others in a tetrahedral pattern [23]. The silicon dioxide lattice is a diamond lattice in which each bond between tetrahedrally coordinated sites has been replaced by a 2-coordinated site. The average coordination number per site on this lattice is $(4 + 2 + 2)/3 = 2.67$.

2.2. (10,3)-a oxide

The (10,3)-a lattice is part of a larger family of 3-coordinated lattices. The lattices in this family go by a number of names, but perhaps the most exhaustive exploration of this family of lattices was by Wells, who coined the name (10,3) [22]. The 3 reflects the three-fold coordination of the sites. The number 10 reflects the fact that if one were to make a circuit on the lattice, traveling site-by-site and visiting no site more than once before the return to the starting point, the shortest path would be a 10-gon. The -a reflects the fact that there are seven lattices in this family, named alphabetically: (10,3)-a, (10,3)-b, etc. In its most symmetric realization, the (10,3)-a lattice is a bcc lattice with a 4-atom basis, each site having three neighbors. This lattice is of interest for a number of reasons, including the fact that there are real materials with this structure (e.g. block copolymers [24–26], molecular magnets [27, 28] and even butterfly wings [29]). Additionally, it has unusually high symmetry, possessing a property known as ‘strong isotropy’ [30], shared with only one other 3D lattice (diamond). The structure of (10,3)-a is illustrated in our previous paper on this subject [16].

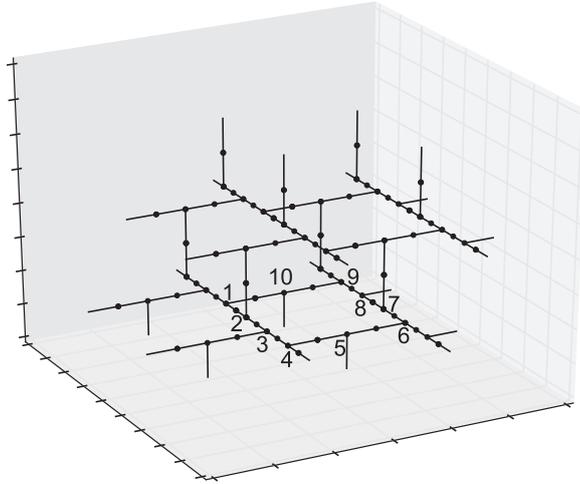


Figure 3. The (10,3)-a oxide lattice, with bond angles deformed to fit onto a cubic grid for convenience. We number ten of the 3-coordinated sites (but not the 2-coordinated sites joining them) to show that the shortest circuit along the underlying (10,3)-a lattice is a 10-gon.

The oxide form that we will study for this lattice is one in which a 2-coordinated site is inserted between each 3-coordinated site. If we denote the 2-coordinated sites as O (for oxygen) and the 3-coordinated sites as X, the stoichiometric formula of this structure is X_2O_3 , but it is important to note that this is *not* the typical structure of a Group III oxide (e.g. the most common form of aluminum oxide has a coordination number higher than 3 [31]). For our purposes here, (10,3)-a oxide is of interest for being a convenient lattice with a low coordination number. For each pair of 3-coordinated sites there are three 2-coordinated sites, giving an average coordination number of $(2 \cdot 3 + 3 \cdot 2)/5 = 2.4$. We illustrate it in figure 3, with bond orientations deformed to fit the lattice onto a cubic grid for convenience in enumerating sites.

2.3. (10,3)-b oxide

The (10,3)-b lattice is similar to (10,3)-a, in that the shortest circuit that returns to a site is a 10-gon and that the primitive cell has four atoms. The effective coordination number of the oxide is again 2.4. However, the lattice contains an extra structural degree of freedom. Even if all bond angles are 120 degrees and all bonds are equal length (i.e. a highly symmetric realization of the lattice), we can continuously deform the lattice in a manner that uniformly changes the spacing between planes without altering any bond lengths or angles. In the maximally symmetric case, the lattice is body-centered tetragonal with a four-atom basis. If, however, we compress the lattice to decrease the spacing between planes, it begins to look like a 3D generalization of a honeycomb lattice, being a stacking of interwoven honeycomb planes. For this reason, the (10,3)-b lattice has been referred to as the ‘hyper honeycomb’ lattice and has attracted some interest in the study of spin systems [32]. We will consider an oxide form which, again, has a 2-coordinated site along each bond. We illustrate it figure 4, with bond orientations deformed to fit the lattice onto a cubic grid for convenience in enumerating sites.

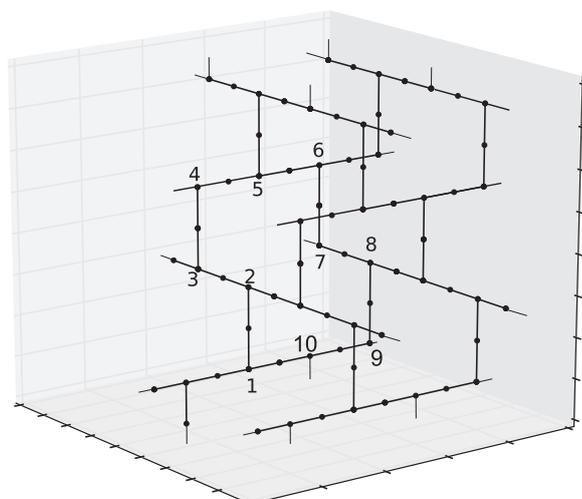


Figure 4. The (10,3)-b oxide lattice, with bond angles deformed to fit onto a cubic grid for convenience. We number ten of the 3-coordinated sites (but not the 2-coordinated sites joining them) to show that the shortest circuit along the underlying (10,3)-b lattice is a 10-gon.

2.4. Cubic oxide

Cubic oxide is a simple cubic lattice (6-coordinated sites) with 2-coordinated oxygen sites along the bonds between the 6-coordinated sites. There are six oxygen sites bonded to each 6-coordinated site. The oxygen sites are shared between two neighbors, so the stoichiometric formula is XO_3 and the average coordination number is $\bar{z} = (1 \cdot 6 + 3 \cdot 2) / 4 = 3$. While we have studied the case of $z = 3$ in our previous work on 3-coordinated lattices, this case was included to see if there are significant differences between a homogeneous lattice (all sites the same coordination number) and an oxide with a different underlying structure but the same average coordination number.

3. Computational methods

3.1. The Newman–Ziff algorithm

We determined p_c with the algorithm of Newman and Ziff [5]. We described our implementation in previous work [16]. In brief, the Newman-Ziff algorithm occupies sites or bonds on a lattice in a random order. When a new site (or bond) is occupied, the program checks to see if it borders an existing cluster of sites (or bonds). If so, it joins that cluster. If the new site (or bond) bridges two existing clusters, the clusters are merged. Finally, if the occupation of a new site (or bond) joins two parts of an existing cluster and causes them to wrap completely around, then percolation has occurred and the program moves on to randomly occupy sites or bonds on a new, fresh lattice. By repeating this process N_L times, one can get the fraction R_L of lattices of linear dimension L (i.e. number of unit cells in the system is L^3) that wrap when a given number n of the sites are occupied.

In order to obtain wrapping probability R_L as a function of site occupation probability p , one convolves $R_L(n)$ with the binomial distribution:

$$R_L(p) = \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} R_L(n) \quad (2)$$

The convolution amounts to a weighted sum over all possible realizations of a lattice in which sites are occupied with probability p . For each possible occupation number we multiply the probability of that occupation number occurring (from the binomial distribution) by the wrapping probability for that occupation number.

The plot of $R_L(p)$ has a steep rise at the percolation threshold p_c and one could obtain a reasonable estimate of p_c simply by looking for the point on the graph with the steepest slope. However, one can obtain a higher precision estimate by comparing plots of $R_L(p)$ for several different values of the linear dimension L . The percolation threshold is the point at which the wrapping probability crosses over from 0 to 1 and the width of this cross-over region gets smaller as L increases. Consequently, above p_c the wrapping probability increases as L increases and below p_c the wrapping probability decreases as L increases. If we make a plot of R_L versus L for different site occupation probabilities, this plot will be flattest at $p = p_c$. This method has been used to determine p_c by us and others in previous work [16, 33].

3.2. The uncertainty in the percolation threshold

There is a straightforward way to determine the uncertainty in an estimate of p_c . If one repeatedly generates N_L lattices with the same fraction of occupied sites, one would expect the standard deviation of the fraction that wraps to be given by the binomial distribution: $\sqrt{R_L(1-R_L)/N_L}$. This is the magnitude of vertical fluctuations in the R_L versus p graph, approximately 3% for simulations of $N_L = 10^3$ lattices wrapping with probability $R_L \approx 0.5$ (the numbers used here). The figures below do indeed exhibit vertical fluctuations of that order.

To go from vertical fluctuations to horizontal fluctuations (i.e. the effect on the estimate of p_c), one must divide by the slope of the R_L versus p graph, giving:

$$\delta p_c = \sqrt{\frac{R_L(1-R_L)}{N_L}} \bigg/ \frac{dR_L}{dp} \quad (3)$$

By way of comparison, when we generated $N_L = 10^3$ lattices of size $L^3 = 128 \times 128 \times 128$ unit cells, typically with four or more sites (depending on the lattice) per unit cell, this amounted to producing of order 10^{10} random numbers, which should give uncertainties of order 10^{-5} or larger. For the cases shown below, uncertainties were estimated to be between $2 \cdot 10^{-5}$ and $5 \cdot 10^{-5}$, consistent with the number of random numbers generated.

We convolved our $R_L(n)$ data with the binomial distribution twice. On the first pass, we worked with a coarse-grained distribution, varying the site occupation probability p in steps of $1/(\text{smallest lattice size})$. We looked for the approximate intersection of the R_L versus p curves to get an approximate p_c and used the values of R_L and dR_L/dp to get an approximate uncertainty in p_c . After that, we again convolved $R_L(n)$ with

Table 1. Site percolation thresholds for oxides studied here. Uncertainties in p_c estimates are given in parentheses and refer to the last two digits.

Lattice	Average neighbors per site	p_{cZ1}	p_c (site)
(10,3)-a oxide	2.4	2.246	0.748 713(22)
(10,3)-b oxide	2.4	2.236	0.745 317(25)
Silicon dioxide	2.66...	2.555	0.638 683(35)
Cubic oxide	3	3.148	0.524 65(5)

the binomial distribution, this time varying p in steps of the estimated uncertainty. After the second convolution, we looked for the value of p that made $R_L(p)$ flattest (i.e. smallest slope in a least squares fit) as a function of L , to get a better estimate of p_c and its uncertainty.

Using this method for determining p_c and the uncertainty in p_c , we previously [16] determined the site percolation threshold of the 3D simple cubic lattice to be in close agreement with the literature value [34]. As a further check on our work, before computing the percolation threshold of silicon dioxide we used simulations to determine the site and bond percolation thresholds of the diamond lattice, getting results in good agreement with the most precise available literature values [35]. Besides confirming the reliability of our implementation of the Newman–Ziff algorithm, this also gives us confidence that our code correctly represents the silicon dioxide lattice, as the code for silicon dioxide was based on the test code for the diamond lattice (due to the close relationship between the lattices).

4. Computational results for site percolation thresholds of oxides

Figures 5–8 show R_L versus L for silicon dioxide, cubic oxide, (10,3)-a oxide and (10,3)-b oxide. For each type of lattice we generated $N_L = 10^3$ cases. Each figure shows plots for selected values of p , spaced by intervals of the uncertainty (as computed from equation (3)). There are fluctuations in the graphs of R_L versus L , but they are of order $\sqrt{R_L(1-R_L)/N_L}$ as discussed above and the mean values (≈ 0.45) of the wrapping probability R_L at the percolation threshold are very close to values found at p_c in other investigations of 3D site percolation [33]. For a given value of L , all values of R_L fluctuate in the same direction and by approximately the same amount (irrespective of the value of p) because they are derived from the same set of simulated lattices. The percolation thresholds of these oxides are summarized in table 1.

With these numbers in hand, we can compare the computed percolation thresholds with the predictions of power-law scaling. As discussed above, we have at least two plausible methods for quantifying the average coordination number on a lattice and each measure, when used in the power-law, will give a different prediction for the site percolation threshold. In figure 9, we show the errors produced by each method for the four oxides studied, as well as the octagonal lattice (which has mixed coordination number and is discussed below in section 6). For comparison, we also show the errors for several well-known uniform lattices (all sites with same coordination number). Quantifying average coordination number according to the average number of bonds

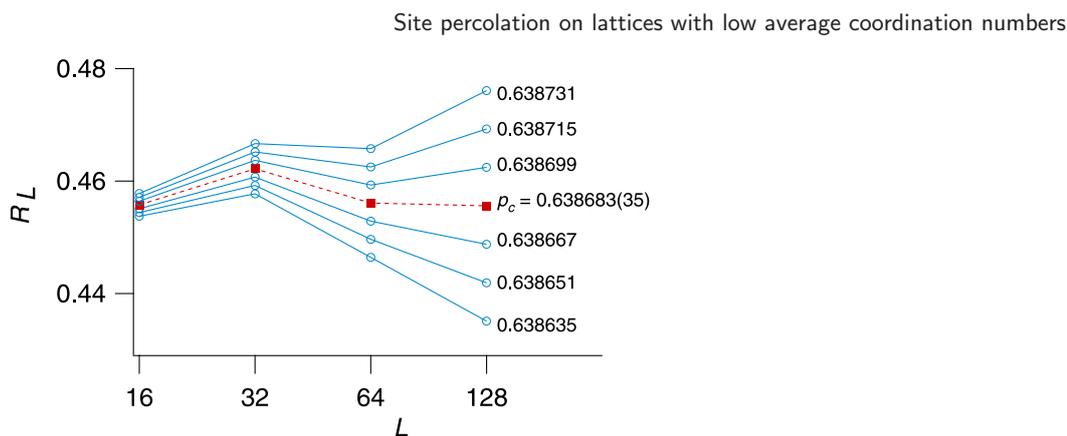


Figure 5. Wrapping probability R_L versus L for site percolation on the silicon dioxide lattice, for different occupation probabilities p . The p that produces the flattest overall trend (dashed red line) is taken to be the percolation threshold p_c . At p_c , we generate 10^3 lattices with wrapping probability approximately 0.46, giving rise to fluctuations with standard deviation $\sqrt{0.46(1-0.46)} / 10^3 \approx 0.016$. The fluctuations in this graph are smaller than one standard deviation at p_c .

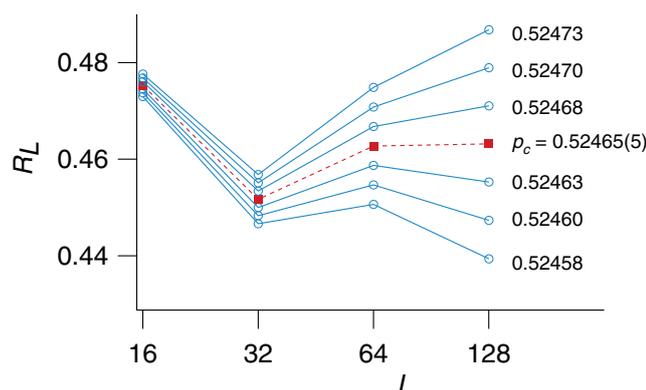


Figure 6. Wrapping probability R_L versus L for site percolation on the cubic oxide lattice, for different occupation probabilities p . The p that produces the flattest overall trend (dashed red line) is taken to be the percolation threshold p_c . At p_c , we generate 10^3 lattices with wrapping probability approximately 0.46, giving rise to fluctuations with standard deviation $\sqrt{0.46(1-0.46)} / 10^3 \approx 0.016$. The fluctuations in this graph are approximately one standard deviation at p_c .

available to a high-coordinated site improves the predictions by at least an order of magnitude for each oxide. When we then plot p_c as a function of $z - 1$ we see that all of the oxides are very close to the same line as other lattices in figure 10.

Interestingly, the errors for the oxides are actually comparable to or smaller than the errors for most of the regular, higher-coordinated lattices. The errors for cubic oxide and silicon dioxide are $\approx 3 \cdot 10^{-4}$ and $\approx 1.5 \cdot 10^{-3}$ respectively, smaller than the errors that Galam and Mauger obtained when they tried to derive effective coordination numbers for uniform 3D lattices [8]. The results are less impressive for the (10,3) oxides, but are still a definite improvement (order of magnitude reduction in error) over the results obtained by using an arithmetic average coordination number. Even

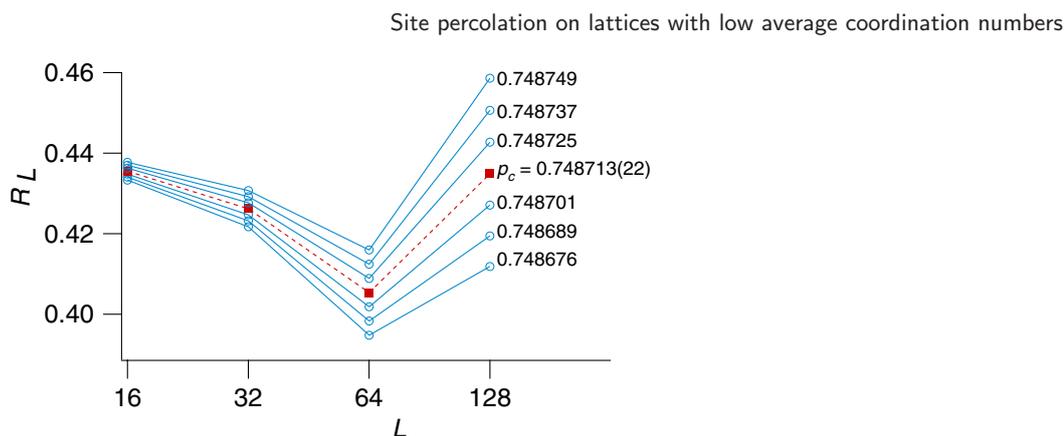


Figure 7. Wrapping probability R_L versus L for site percolation on the (10,3)-a oxide lattice, for different occupation probabilities p . The p that produces the flattest overall trend (dashed red line) is taken to be the percolation threshold p_c . At p_c , we generate 10^3 lattices with wrapping probability approximately 0.44, giving rise to fluctuations with standard deviation $\sqrt{0.44(1-0.44)} / 10^3 \approx 0.016$. The fluctuations in this graph are approximately two standard deviations at p_c .

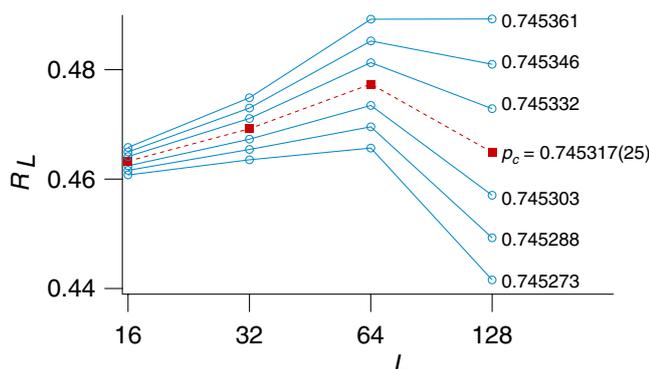


Figure 8. Wrapping probability R_L versus L for site percolation on the (10,3)-b oxide lattice, for different occupation probabilities p . The p that produces the flattest overall trend (dashed red line) is taken to be the percolation threshold p_c . At p_c , we generate 10^3 lattices with wrapping probability approximately 0.46, giving rise to fluctuations with standard deviation $\sqrt{0.46(1-0.46)} / 10^3 \approx 0.016$. The fluctuations in this graph are approximately one standard deviation at p_c .

for the lowest- z oxide, errors are of the same order of magnitude as the errors obtained by Galam and Mauger for uniform 3D lattices of higher coordination number. The fact that the formula of Galam and Mauger happens to be accurate for some lattices is not surprising; what is more interesting is that the formula remains reasonably accurate when one applies it to site-bond problems. The good agreement with power-law scaling for an effective z as low as 2.246 is especially significant in light of the fact that for the higher-coordinated uniform lattices the coordination number is unambiguously defined, whereas there are multiple plausible definitions for the average coordination number of an oxide.

Site percolation on lattices with low average coordination numbers

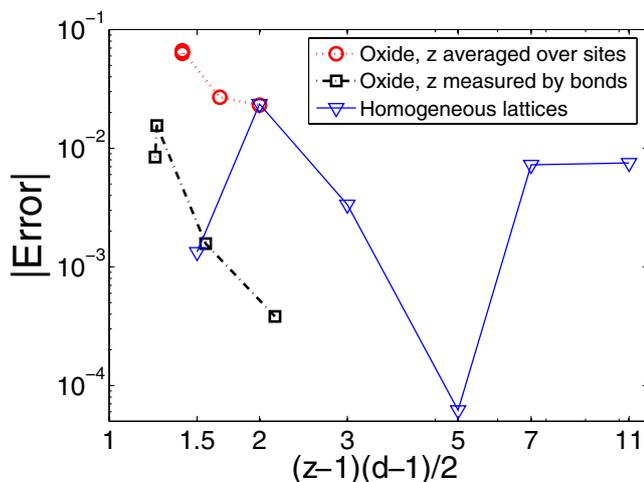


Figure 9. Absolute value of the error in the prediction of the approximate power-law formula, as a function of coordination number or (for oxides) average coordination number. The oxides are (from left to right) (10,3)-b oxide, (10,3)-a oxide, SiO₂ and cubic oxide. The six regular lattices are (from left to right) 2D kagomé [36], (10,3)-a [16], diamond [35], simple cubic [34], body-centered cubic [34] and face-centered cubic [37]. The factor of $(d - 1)/2$ is included in the horizontal axis to enable comparisons between 3D lattices and the 2D kagomé lattice.

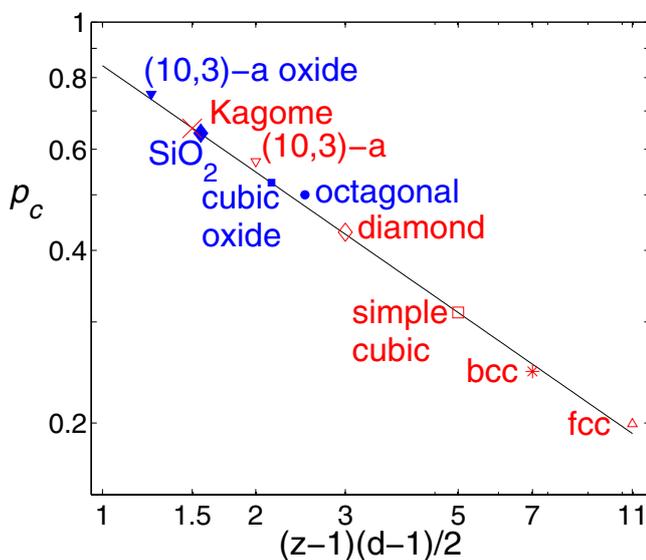


Figure 10. Log-log plot comparing percolation thresholds of different lattices. Lattices with uniform coordination numbers are shown in red and mixed coordination numbers are shown in blue. We include here the 2D octagonal lattice (discussed in section 6). The black line shows the power-law scaling relation from equation (1), with p_0 and a from the second universality class identified by Galam and Mauger. The horizontal scale includes a factor of $(d - 1)/2$ to enable comparisons between 3D lattices and the 2D kagomé and octagonal lattices. For lattices with variable numbers of nearest neighbors, z is the average number of connections between high-coordinated sites at p_c .

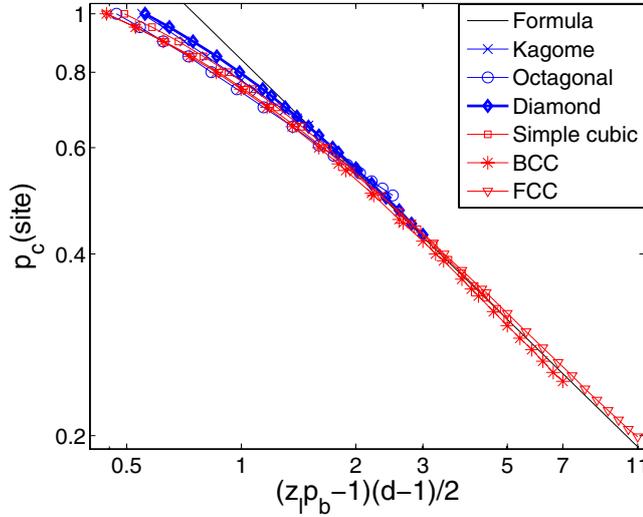


Figure 11. Site percolation threshold (in site-bond percolation) as a function of mean number of available bonds $z_1 p_b$ and dimension d for the universality class of 3D lattices (and also 2D kagomé lattices) identified by Galam and Mauger. We include the dimension on the horizontal axis because the formula depends on $(z - 1)(d - 1)$ and the kagomé lattice is 2D. Results for the diamond, octagonal and kagomé lattices are in blue to highlight lattices with low coordination number. The black line shows the power-law scaling relation from equation (1), with p_0 and a from the second universality class identified by Galam and Mauger.

5. Site-bond percolation as a site percolation problem with low coordination number

We do not have to restrict our attention to oxides if we want to study low coordination numbers. We can also study site-bond percolation problems, in which (as discussed above) sites are occupied with probability p_s and bonds with probability p_b . One can hold the bond occupation probability fixed and vary the site occupation probability (or vice-versa) to see when a wrapping cluster forms and thereby determine the site percolation threshold as a function of bond occupation probability p_b (or vice-versa). Removing some of the bonds reduces the average coordination number from z_1 (the coordination number of the underlying lattice) to $p_b z_1$.

In figure 11 we show plots of p_c versus $p_b z_1$, using data from Tarasevich and van der Marck [21]. We considered several lattices that Galam and Mauger conjectured to fall into the same universality class. The right end of each data series lies close to the line representing the power law of Galam and Mauger, as well as the 2D octagonal lattice (discussed below). The agreement ultimately breaks down at sufficiently small effective coordination numbers, because eventually the problem of constructing a wrapping cluster is dominated by the low number of occupied bonds and scaling relations valid for site percolation no longer apply. Nonetheless, for each lattice considered, the site percolation threshold initially follows the power-law scaling relation as some of the bonds are removed. Quantitative agreement is confirmed by examining the errors in figure 12. The mere fact that the formula of Galam and Mauger works in these cases

Site percolation on lattices with low average coordination numbers

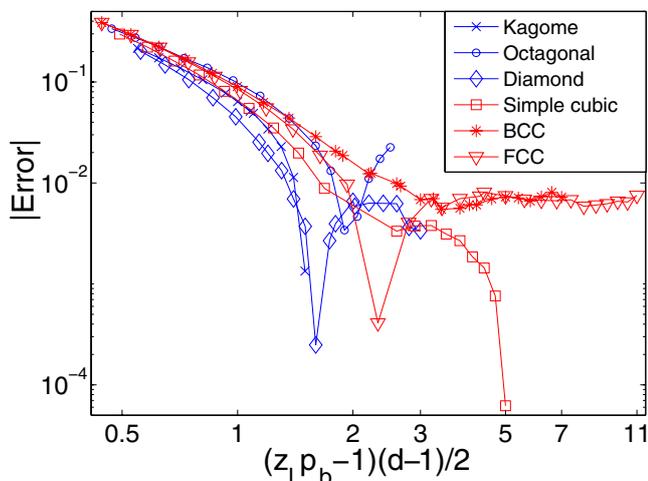


Figure 12. Difference between prediction of power-law scaling and site percolation threshold as a function of average coordination number in site-bond calculations.

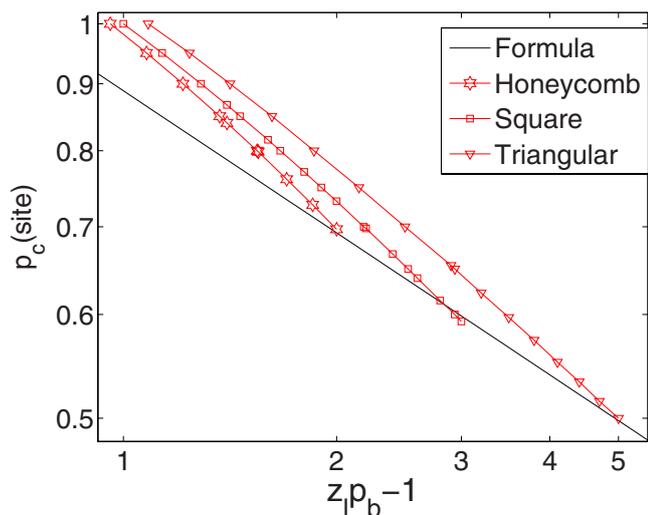


Figure 13. Site percolation threshold (in site-bond percolation) as a function of mean number of available bonds $z_1 p_b$ and dimension d for the universality class of 2D honeycomb, square and triangular lattices identified by Galam and Mauger. The black line shows the power-law scaling relation from equation (1), with p_0 and a from the first universality class identified by Galam and Mauger.

(which have been conjectured to belong to a universality class) is less interesting than the fact that the formula continues to work for those same cases when we generalize from site percolation to site-bond percolation.

However, when we performed the same analysis for the universality class of 2D lattices identified by Galam and Mauger (honeycomb, triangular and square) [7], the results are not well-approximated (even for $p_b \approx 1$) by the power-law scaling of site percolation threshold. We have no good explanation for this phenomenon. It cannot be a consequence of dimensionality, as the 2D kagomé lattice results follow

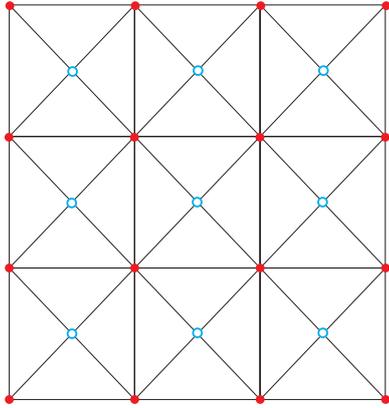


Figure 14. Octagonal lattice, often called the ‘Union Jack’ lattice, with a mix of 8-coordinated (solid red) and 4-coordinated (open blue) sites.

the power-law scaling behavior of regular 3D lattices. While the concept of two distinct universality classes at low dimension has been met with important objections [10, 17], the differences between figures 11 and 13 show that lattices that (approximately) follow a common scaling law for pure site and bond percolation also (approximately) also follow the same scaling law for mixed site-bond percolation. While the universality classes proposed by Galam and Mauger have significant defects (e.g. no criterion to predict which lattices should belong to which class), this difference in scaling behavior suggests that there may be some underlying phenomenon meriting further study. It is worth noting that Ziff and Gu have developed a useful and reasonably accurate (better than 3%) approximate formula for site-bond percolation on the honeycomb lattice [12], but we are not aware of any generalization that we can use for other 2D lattices.

6. Discussion

The measures we considered here for average coordination number are not the only possible approaches. Galam and Mauger proposed that one could define an effective coordination number as the value of z that minimizes the sum of the errors in the site and bond percolation thresholds (with errors defined as the difference between the actual percolation threshold and the predictions of power-law scaling). However, this is an after-the-fact definition of effective coordination number, requiring knowledge of the true percolation threshold. One cannot derive this effective coordination number from a direct examination of lattice geometry, but only from already knowing the percolation threshold. Our approach, in which we define $z_1 p_c$ as the effective coordination number at the percolation threshold, can be used to obtain a prediction of p_c without *a priori* knowledge of the percolation threshold. If one uses power-law scaling, one gets an implicit formula for an oxide’s site percolation threshold p_c :

$$p_c = p_0 ((d-1)(z_1 p_c - 1))^{-a} \quad (4)$$

This equation can be solved for p_c , as long as one knows z_1 , d , p_0 and a .

We can generalize this procedure. Consider a more complicated lattice, such as the octagonal lattice (figure 14) with site percolation threshold $p_c^{(s)} = 0.5$ (because it is fully triangulated) [18]. We consider the octagonal lattice because (1) its combination of site and bond [18] percolation thresholds make it a plausible candidate for being in the same universality class as the kagomé lattice [38] and (2) its structure of mixed coordination numbers is more complex than the oxides considered above, but is nonetheless simple to study. Let us assume that formation of a percolating cluster is dominated by the 8-coordinated sites and that the 4-coordinated sites primarily serve to facilitate links between 8-coordinated sites. Each 8-coordinated site has direct bonds to four other 8-coordinated sites, as well as four 4-coordinated sites. Occupation of these other 4-coordinated sites is not the only way to reach other 8-coordinated sites, but we can begin by trying to ‘average out’ the 4-coordinated sites, modeling this in a manner analogous a site-problem.

In our approximation, where we replace 4-coordinated sites with bonds, at the percolation threshold, $4p_c$ of the 4-coordinated neighbors will be occupied and permit access to 8-coordinated neighbors. Additionally, there are direct bonds to four other 8-coordinated sites. The average coordination number is thus $4 + 4p_c$. If we assume the power-law scaling relation to hold, we get:

$$p_c = p_0((d-1)(4+4p_c-1))^{-a} \quad (5)$$

This is an implicit equation for p_c . More importantly, it was derived by taking into account features of the lattice beyond nearest neighbors, addressing one of the common criticisms of the Galam-Mauger power law. If we solve equation (5) numerically we get that the site percolation threshold is 0.4818. This is reasonably close to the exact site percolation threshold of $1/2$, but still not resounding agreement. However, when we use this prediction of the site percolation threshold to compute an effective coordination number ($4 + 4p_c = 5.93$) and then use that in Galam and Mauger’s formula for the bond percolation threshold, we get the prediction $p_c^{(b)} = 0.3247$, which agrees with the bond percolation threshold determined from Monte Carlo simulations ($p_c^b = 0.3237$) to 0.3%. While our inclusion of the octagonal lattice in the same universality class as kagomé is just conjecture, the site bond results for octagonal in figure 11 follow the same trend as kagomé and the 3D lattices, suggesting that its inclusion in this conjectured universality class is a hypothesis worthy of further study.

Of course, our approach to ‘averaging out’ lower-coordinated sites is *ad hoc* and gives no obvious prescription for more general lattices. We only present it as the beginning of an idea that might be generalized to more complicated lattices: Treating the higher-coordinated sites as the key players in the formation of a percolating cluster and the lower-coordinated sites as providing an average number of bonds between the higher-coordinated sites. By removing the lower-coordinated sites from explicit consideration, one is removing the shortest length scales from the analysis, bringing in ideas analogous to renormalization group calculations. However, renormalization treatments of percolation do not assume compliance with an empirical power law derived from Monte Carlo simulation results, unlike our use of the Galam Mauger formula. Nonetheless, power laws are closely related to the idea of scale invariance, raising the question of whether our approach to oxides and the octagonal lattice might have connections to renormalization ideas. However, given that there are demonstrated examples of lattices for

which our approach does *not* support a power-law relationship between site percolation threshold and average coordination number, a more rigorous exploration of these ideas would have to provide some criterion for identifying the lattices that can be treated by this approach. Criteria that relate lattice topology to properties of percolating clusters seem especially promising for further insight [11].

7. Conclusions

In conclusion, we have shown that Galam and Mauger's conjectured power-law relationship between site percolation threshold and average coordination number (equation (1)) holds for site percolation on a number of lattices with average coordination number less than 3. These lattices are closely analogous to oxide materials. The quantitative accuracy of the power-law scaling relationship depends on how the average coordination number is defined and measured, with better agreement when we define average coordination number as the average number of available bonds between higher-coordinated sites.

Our results suggest a two-fold utility to the power-law relationship conjectured by Galam and Mauger: First, while it is already known that the power-law relationship predicts (usually to a precision of a few percent or better) the standard site and bond percolation thresholds of many lattices in rather arbitrarily-defined classes, we show here that it can also be applied to mixed site-bond problems on one (admittedly arbitrarily-defined) class of lattices. The relationship also works reasonably well for site percolation on lattices with mixed coordination number (e.g. octagonal). Second, when one uses a suitable definition of average coordination number (a definition that measures the connection between higher-connected links) the formula of Galam and Mauger becomes an implicit formula for the site percolation threshold, one that can take into account neighbors beyond just the nearest ones.

Finally, although there are some key cases in which our approach to site-bond problems fails to give good agreement between simulation results and the conjectured power-law scaling behavior, the relevant lattices are those that had previously been conjectured to fall into a distinct universality class. While there are still significant conceptual problems with the power-law scaling formula and the conjectured universality classes, our results suggest that a re-examination is merited, to see if there are ways to refine these conjectures to take into account additional features of the lattice structure and refine estimates of percolation thresholds.

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