Dependence of percolation thresholds on lattice connectivity

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We investigate site percolation on lattices with directed bonds. Numerical simulations in which the lattice coordination number of the percolation lattices is systematically varied show that the inverse of the percolation threshold depends approximately linearly on the lattice coordination number. We show that this linear relationship is due to a similarity of percolation clusters in lattices for different coordination numbers. We compare this relationship to results obtained by Flory [*Principles of Polymer Chemistry* (Cornell University Press, Ithaca, New York, 1953), Chap. IX] in the study of gelation processes and discuss its general applicability for related percolation models.

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Starting with the work of Broadbent and Hammersley [1], percolation phenomena have been studied as models for a variety of physical processes. The various applications have led to the study of percolation transitions on different lattices (quadratic, hexagonal, ...) and under a variety of conditions, such as site percolation, bond percolation, and correlated percolation. These studies have led to a wealth of data about critical probabilities and critical exponents which characterize the percolation transitions [2,3].

In these studies the same sets of critical exponents appeared in different percolation transitions. This led to the classification of percolation transitions into universality classes according to their sets of critical exponents. The origin of the critical exponents in percolation and other phase transitions continues to attract widespread interest [4,5].

Comparatively little effort has been spent on classifying the percolation thresholds. In Flory's gelation theory [6], which can be understood as percolation on a Cayley tree, the gelation threshold p_c was found to depend on the lattice coordination number f as

$$p_c^{-1} = (f-1). \tag{1}$$

This formula is derived from the simple requirement that a cluster of molecules can only be of infinite size and thus form the gel phase if every molecule connected to this cluster by one of its f possible bonds continues the cluster through at least one of its $(f-1)$ remaining bonds. Many subsequent refinements, mostly from scientists closer to an experimental approach, have led to the introduction of correction factors that take into account intramolecular reactions or dilution effects but leave the basic mean-field-theory approach unaltered.

For example, Kilb's calculations [7] and Stepto's experiments [8] suggest expanding Flory's formula (1) to

$$p_c^{-1} = (1-\lambda)(f-1), \tag{2}$$

where λ describes the fraction of intramolecular reactions. These refined theories usually allow quantitative predictions of the gelation transition.

The percolation-theory approach [9,10], on the other hand, focuses less on a quantitative prediction of the threshold but more on a qualitatively correct description of the critical behavior in the vicinity of the percolation transition. By replacing the Cayley tree by more realistic two- or three-dimensional lattices, one obtains more realistic critical exponents than those obtained by mean-field theory. Coniglio, Stanley, and Klein [11] also included dilution and correlation effects in their percolation model of the gelation process. However, the relative lack of success in predicting qualitatively the gelation threshold might be due to the restricted choice of lattices that have so far been used for percolation studies.

The lattices used for percolation studies were usually chosen out of a small pool of simple lattices. The prevalence of quadratic lattices with nearest-neighbor-only interactions is, e.g., more readily explained in terms of their ease of manipulation than in terms of their specific relevance to polymer gelation.

Since, as mentioned earlier, the critical exponents are fairly insensitive to details of the lattice geometry, this approach was justified when the investigations focused on critical exponents. For quantitatively meaningful results for the percolation transition, however, more attention has to be paid to the details of the lattice geometry.

In our investigations we explore systematically how percolation thresholds depend on the lattice connectivity. We initially focused on directed site percolation. (Using *directed* bonds simplifies the cluster-counting procedure considerably since it then only requires one single sweep through the lattice.) In our lattices, every site (i,j) was connected to z sites $(i-1,j-(z-1)),\ldots,(i-1,j)$ through incoming directed bonds and to z sites $(i+1,j),\ldots,(i+1,j+(z-1))$ through outgoing directed bonds. (For $z=2$, this geometry is equivalent to the quadratic lattice with directed bonds studied by Kinzel and Yeomans [12].) Sites denoted by the same first coordinate i will be said to belong to the same *generation* of cells.

Our simulations are carried out as follows: First we fill a fraction p of the sites with *cells* and tag *all* cells in the first generation as *belonging to the cluster*. For every subsequent generation we then tag those cells that can

be reached through directed bonds from tagged cells in the previous generation. In this way we obtain in every generation all the cells that can be reached from cells in the first generation through an uninterrupted chain of directed bonds.

For every generation i, we determine the fraction w_i of sites that are occupied by tagged cells. For values of p below the percolation threshold p_c, w_i will steadily decrease and eventually reach zero. For values of p above the percolation threshold p_c, w_i will decrease from its initial value of p and eventually scatter around its asymptotic value w_∞. This asymptotic value is then identified with the strength of the infinite cluster.

As p approaches p_c from above, the asymptotic value w_∞ decreases to zero. At the same time, the number of generations through which the percolation process has to be iterated to obtain reliable estimates for w_∞ diverges. Therefore, using simulations of lattices of a given finite size, one will not be able to obtain reliable values for very small w_∞.

In our simulations we used lattices of 50 000 sites per generation and iterated up to 200 000 generations. We then determined the values of p_c and γ which would result in the best fit of the data to the form

$$w_\infty(p) = (p - p_c)^\gamma. \tag{3}$$

We applied this procedure to a set of different lattice geometries that were characterized by varying numbers of bonds z. The resulting percolation thresholds for z in the range from 1 to 8 are shown in Table I. For all z, we obtained values of $\gamma = 0.29 \pm 0.02$ that agree for $z = 2$ with the value obtained in [12].

Columns 3 and 4 of Table I show the inverse value of the percolation threshold as well as the increment $\Delta(z) = 1/p_c(z) - 1/p_c(z-1)$. The convergence of $\Delta(z)$ to the value of 0.445 ± 0.003 suggests the empirical formula for the percolation thresholds,

$$\frac{1}{p_c(z)} \approx 0.518(3) + 0.445(3)z, \tag{4}$$

with significant deviations only for small n, i.e., $n = 1, 2, 3$.

We now want to explore the origin of the linear relationship expressed in (4) by calculating the strength of the cluster in generation i through a recursion relation.

TABLE I. Thresholds for site percolation with directed bonds. z denotes the number of connections per site. $\Delta(z)$ has been calculated by $\Delta(z) = 1/p_c(z) - 1/p_c(z-1)$.

z	$p_c(z)$	$1/p_c(z)$	$\Delta(z)$
1	1	1	
2	0.7052(2)	1.4180	0.4180
3	0.5387(3)	1.8563	0.4383
4	0.4351(3)	2.2983	0.4420
5	0.3645(3)	2.7435	0.4452
6	0.3135(3)	3.1898	0.4463
7	0.2754(3)	3.6311	0.4413
8	0.2452(3)	4.0783	0.4472

For any site to belong to the cluster, it has to be occupied by a cell, and at least one parent site in the previous generation has to belong to the cluster. The probability $w_{i+1,j}$ that site j in generation $(i+1)$ belongs to the cluster can be expressed in terms of the probabilities $w_{i,k}$ for the sites in the previous generation, of the cell concentration p, and of the number of parent sites z

$$w_{i+1,j} = p\left(1 - \prod_{k=0}^{k=z-1}(1 - w_{i,j-k})\right). \tag{5}$$

(The second index in $w_{i+1,j}$ indicates that this probability refers to one specific cell j. If this second index is missing, the quantity is to be understood as the average over all cells of a generation.) The product term on the right-hand side expresses the probability that all parent sites are not cluster sites. If we neglect any correlation effects (i.e., $w_{i,j} = w_{i,j'} = w_i$) and use the self-consistency condition ($w_{i+1} = w_i = w_\infty$) we can transform Eq. (5) to

$$p = \frac{w_\infty}{1 - \prod_{k=0}^{k=z-1}(1 - w_\infty)}. \tag{6}$$

We then obtain the percolation threshold p_c by letting w_∞ approach zero from above, i.e.,

$$p_c = \lim_{w_\infty \to 0} p = \lim_{w_\infty \to 0} \frac{w_\infty}{1 - \prod_{k=0}^{k=z-1}(1 - w_\infty)}$$

$$= \lim_{w_\infty \to 0} \frac{w_\infty}{1 - (1 - z w_\infty + \cdots)} = \frac{1}{z}. \tag{7}$$

We thus obtain again the Flory result of Eq. (1) in that the percolation threshold equals the inverse of the number of outgoing bonds.

We now take into account correlation effects. For this purpose, we introduce conditional probabilities when calculating the product probability that none of the parent sites are cluster sites. The probability that parent site $(i, j+k')$ is not a cluster site will be lowered if we know that the parents $(i, j+1), \ldots, (i, j+k'-1)$ are noncluster sites. This can be expressed by setting

$$w_{i,j+k} = c_{k,z} w_i \tag{8}$$

with $c_{0,z} = 1$ and $0 < c_{k,z} < 1$ for $k > 0$. Note that the $c_{k,z}$ are $(k+1)$-site correlation functions. Inserting these correlation coefficients into Eq. (5) and solving for p_c, one obtains

$$\frac{1}{p_c(z)} = \sum_{k=0}^{z-1} c_{k,z} = z\bar{c}(z), \tag{9}$$

where

$$\bar{c}(z) = \frac{1}{z}\sum_{k=0}^{z-1} c_{k,z} \tag{10}$$

is the average of the correlation coefficients.

It should be pointed out that these coefficients $c_{k,z}$ do not only depend on k and z, but also on w_i and p.

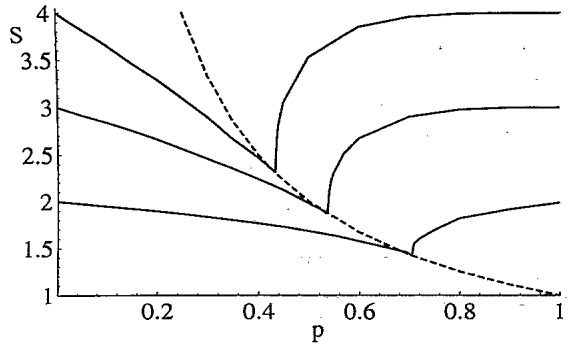

FIG. 1. $S=\sum_{k=0}^{n-1} c_{k,z}(p)$ (continuous curves) for $z = 2, 3, 4$, and $f(p) = 1/p$ (broken curve) as a function of the lattice occupancy p. These curves intersect at the critical probabilities $p_c(z)$ for the respective z.

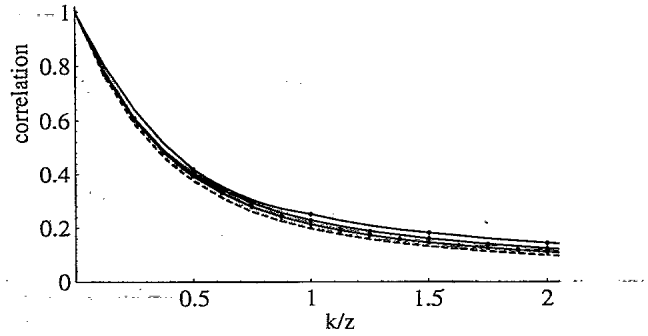

FIG. 2. Correlation values $c_{k,z}$ plotted as a function of k/z. Starting with the uppermost line, the lines connect correlation values pertaining to z=2, 4, 8, obtained from simulations using $p = 0.704, 0.434, 0.2445$, respectively. The dashed curve approximates the asymptotic function $c^*(k/z)$.

In the present investigation, we are only interested in the values $c_{k,z}$ for $w_i = w_\infty$. In simulations, we thus look at the percolation cluster in sufficiently high generations, where the properties of the cluster no longer depend on the properties of the cluster in generation 1. The dependence of $\sum_{k=0}^{z-1} c_{k,z}$ on the cell concentration p is shown in Fig. 1 for $z = 2, 3, 4$. Notice that for p close to 0 or 1, $\sum_{k=0}^{z-1} c_{k,z} \approx z$, i.e., correlations do not play a role in nearly empty or nearly fully occupied lattices. Correlations are most significant around $p \approx p_c$. At $p = p_c$, the curves for $\sum_{k=0}^{z-1} c_{k,z}$ intersect the broken curve $f(p) = 1/p$, thus confirming the first equality of Eq. (9).

We now focus on the values of the correlation coefficients for $p = p_c$ and investigate their dependence on k and z. It is reasonable to assume that there must be some similarity between percolation clusters obtained in lattices with different coordination numbers. This similarity should be reflected in a relation between the correlation coefficients for different z.

As shown in Fig. 2, our numerical calculations for $z = 2, 4$, and 8 indeed suggest that for large z the $c_{k,z}$'s depend on k and z only in the combination (k/z) and that we can set

$$c_{k,z} = c^*(k/z). \tag{11}$$

Then, the evaluation of the sums of Eq. (10) can be understood as a Riemann integration over the function $c^*(k/z)$, which uses z strips and in which the value of the function at the lower bound of the integration strip is taken as the value for the whole strip.

For large z, the Riemann sum (10) converges towards the integral over $c^*(k/z)$, which is independent of z. Then, the only remaining z dependence of the percolation thresholds in Eq. (9) will be the linear factor z. The numerical values for the $c_{k,z}$ were obtained for values of p slightly below p_c (0.704 vs 0.7052, 0.434 vs 0.4351, 0.2445 vs 0.2452) in order to obtain convergence in finite time. As a consequence, the correlation values shown in Fig. 2 are slightly higher than their true values for $p = p_c$. In addition, it is to be expected that there are, for small z, some deviations between $c_{k,z}$ and the asymptotic values $c^*(k/z)$. Indeed, Fig. 2 does not show exact overlap for the curves obtained for $z = 2, 4$ or for $z = 4, 8$. To estimate how close the curves connecting the points $c_{k,z}$ are to the asymptotic function $c^*(k/z)$, we evaluated their integral from 0 to 1. The values obtained were $0.490, 0.471, 0.460$ for $z = 2, 4, 8$, respectively. From Eq. (4), the integral of the asymptotic function $c^*(k/z)$ is expected to be 0.445. For comparison, we included a curve (broken line) in Fig. 2 whose integral is 0.445.

We have carried out similar investigations also for percolation on lattices that resemble the Bethe cactus discussed in [13]. Details of these calculations will be reported elsewhere. Here we only note that different species of these cacti are characterized by different correlations, but within a species, we again found a linear relation between the coordination number and the percolation threshold.

It is thus reasonable to assume that an asymptotic linear relationship

$$1/p_c(z) = z\bar{c} \tag{12}$$

will be found in many sets of lattices in which the coordination number is systematically varied.

Finally, we want to comment on different interpretations of the linear dependence between the percolation thresholds and the lattice coordination number as expressed in Eq. (12). From one point of view, this law describes how the percolation threshold decreases when the number of bonds that one site can form increases. Another point of view may be taken when one is interested in the clustering of (macroscopic) particles that can be bonded not through a finite number of bonding sites, but rather at arbitrary points on their surfaces. Such a problem might be modeled through percolation theory by discretizing the surfaces of the particles. The coarseness of the discretization introduces some arbitrariness into the model. However, the asymptotic linear relationship between the percolation threshold and the number of bonding sites then states the very plausible assertion that the density of functional bonds per unit surface area required for percolation becomes independent of the discretization for sufficiently fine-grained discretization.

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