Topological estimation of percolation thresholds

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Abstract. Global physical properties of random media change qualitatively at a percolation threshold, where isolated clusters merge to form one infinite connected component. The precise knowledge of percolation thresholds is thus of paramount importance. For two-dimensional lattice graphs, we use the universal scaling form of the cluster size distributions to derive a relation between the mean Euler characteristic of the critical percolation patterns and the threshold density $p_c$. From this relation, we deduce a simple rule to estimate $p_c$, which is remarkably accurate. We present some evidence that similar relations might hold for continuum percolation and percolation in higher dimensions.

Keywords: topology and combinatorics, classical phase transitions (theory), percolation problems (theory)

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Consider a regular \( d \)-dimensional lattice where a fraction of sites is selected independently with probability \( p \) and deemed ‘black’, with the complementary vertices said to be white. The aggregate of these spatial lattice elements forms a random pattern, which we may partition into clusters after specifying a neighborhood. This simple set-up constitutes the standard model of Bernoullian percolation theory, and is applied to problems as diverse as transport in disordered media, epidemics, and the quark confinement transition in the early universe [1]–[3]. The central result of this theory is the existence of a sharp threshold value \( 0 < p_c < 1 \) in an infinite lattice of dimension \( d > 1 \): when \( p \) increases across \( p_c \), a single infinite cluster appears almost surely and grows in mass with increasing \( p \) beyond \( p_c \) [4]–[6].

Research in percolation theory focussed predominantly on the \textit{universal} critical phenomena showing up in the vicinity of the threshold. On the other hand, for practical application of percolation concepts, it is the specific and \textit{non-universal} value of \( p_c \) which is of primary importance. Exact values of \( p_c \) are known only for special classes of 2D lattices [7]–[12]. In all other cases, values of \( p_c \) are estimated numerically with computer simulations, which often are time consuming, in particular in 3D or higher-dimensional lattices.

Here, we investigate the signature of the percolation transition in the \textit{Euler characteristic} of the spatial pattern formed by the percolating clusters. Its mean value per site, \( \chi(p) \), provides a topological descriptor, which for a lattice \( \Lambda \) turns out to be an exactly calculable finite polynomial in \( p \). For 2D lattices the polynomials \( \chi(p) \) have one non-trivial zero \( 0 < p_0(\Lambda) < 1 \). From the comparison with known threshold values, we observe that \( p_0(\Lambda) \) gives a tight upper bound for \( p_c(\Lambda) \) for many lattices, but we also find exceptions to this rule of thumb. In the case of 3D lattices, each \( \chi(p) \)-polynomial has two
Figure 1. (a) Black clusters partition the white vertices into an aggregate of complementary clusters. For the square lattice, white vertices are connected by lattice bonds and by diagonal bonds across the faces of the lattice. (b) The black and white clusters of size 1 and 2 on the square lattice. The white perimeter sites of a black cluster are connected (and vice versa).

distinct non-trivial zeros which are again slightly larger than the threshold values of the two distinct percolation transitions of black and white clusters.

For 2D lattices, we explain this peculiar ordering of $p_0$ and $p_c$ using the known scaling expression for the critical percolation clusters at $p_c$. Moreover, this approach leads to a surprisingly simple relation which combines via $\chi(p)$ the specific lattice geometry with universal critical percolation features into an accurate parameter-free estimate of percolation thresholds of all 2D lattices considered in this paper. Our work also applies to bond percolation problems when they are reformulated as the equivalent site percolation problem on the covering lattice.

1. The Euler characteristic in percolation theory

The percolation transition is a paradigm of a non-thermal phase transition, where the local merging of black clusters causes an abrupt change in the large-scale connectivity of black vertices. Since the Euler characteristic (EC) is a prominent descriptor of global aspects of spatial patterns, we may expect it to be also a valuable tool in the study of the percolation transition. In this section, we introduce the EC descriptively and discuss its salient features; a more technical but elementary outline can be found in the supplementary notes.

For the time being we consider planar lattices with cyclic boundary conditions. The basic objects in site percolation are clusters of vertices, naturally defined by the connectivity of the host lattice: two black vertices belong to the same cluster if they are joined by a path of black nearest neighbors on the lattice. Moreover, each configuration of black clusters specifies in a natural way an aggregate of white clusters with a complementary neighborhood, which is in general distinct from the black one; it may be visualized by drawing ‘matching’ bonds diagonally across polygonal faces of the host lattice, as illustrated in figure 1(a) for the square lattice. The lattice comprising the vertices of the original lattice and all bonds between neighboring white vertices is called the matching lattice. The complementary connectivities of black and white clusters imply that the white perimeter vertices of black clusters form closed boundaries of holes in white clusters and vice versa, as illustrated for black and white clusters of size one and two in
The percolation thresholds of a lattice $\Lambda$ and its matching lattice $\bar{\Lambda}$ add up to one $[13]$:

$$p_c(\Lambda) + p_c(\bar{\Lambda}) = 1,$$

implying that the black and white clusters are simultaneously critical at $p = p_c$.

Let $g_{st}$ denote the number of black clusters per lattice site with a fixed size $s$ and a fixed number $t$ of perimeter vertices. The mean density of finite black clusters is then given by

$$\bar{n}(p) = \sum_s n_s(p) = \sum_{st} p^t g_{st} \bar{p}^t,$$

where $\bar{p} = 1 - p$ is the density of white vertices, comp. figure 1(b). Correspondingly, the mean density of the complementary finite white clusters reads

$$\bar{n}(\bar{p}) = \sum_s \bar{n}_s(\bar{p}) = \sum_{st} \bar{p}^t g_{st} \bar{p}^t.$$

In their pioneering paper $[13]$ one exact percolation thresholds in two dimensions, Sykes and Essam considered the difference

$$\chi(p) = n(p) - \bar{n}(\bar{p}) = -\bar{\chi}(\bar{p})$$

and found that $\chi(p)$ is a finite polynomial, which they called matching polynomial. This observation enabled them to obtain, for instance, the exact critical probability of site percolation on the ‘self-matching’ triangular lattice from $\chi_{\text{tri}}(p_c) = 0$ at $p_c = \frac{1}{2}$.

When specialized to spatial patterns $P_N$ on a planar lattice with $N$ sites, the definition of the Euler characteristic, $X$, reads

$$X(P_N) = \# \text{clusters of } P_N - \# \text{holes in } P_N.$$  

From comparison of this definition with equation (2), and the observation that complementary (finite) white clusters constitute the holes in black clusters (see above), we see that the matching polynomial $\chi(p)$ may be identified with the mean Euler characteristic per site (MEC) of the black clusters, $\chi(p) = \lim_{N \to \infty} \langle (1/N) X(P_N) \rangle_p$. Equation (2) expresses the fundamental topological invariance of the EC, but the representation as the difference of two infinite series is not convenient for practical computation. For that purpose we employ Euler’s polyhedral formula, which expresses the EC

$$X = \# v - \# e + \# f$$

in terms of the number of black vertices $\# v$, edges joining black vertices $\# e$ and polygonal faces with black boundary $\# f$, respectively. The mean value $\chi(p)$ is now obtained by a simple local calculation. As an example, consider the square lattice: (i) a vertex is black with probability $p$; (ii) the two vertices bounding an edge are black with probability $p^2$, and there are two edges per vertex; (iii) the four vertices surrounding a face are black with probability $p^4$. Hence, we find for the square lattice

$$\chi_{\text{sq}}(p) = p - 2p^2 + p^4.$$  

The graph of $\chi_{\text{sq}}(p)$ is shown in figure 2(a). Analogously, one finds for the triangular lattice $\chi_{\text{tri}}(\bar{p}) = p - 3p^2 + 2p^3$, which has the above-mentioned self-matching property $\chi(p) = -\bar{\chi}(1 - p)$ (see figure 2(b)). Whenever the lattice cells have finite number of boundary vertices, $\chi(p)$ is a finite polynomial.

The graph of $\chi_{\text{sq}}(p)$ in figure 2 is typical for the MEC of 2D lattices. At small values of $p$, black clusters are finite holes in a single infinite white cluster. As long as $p$ is well below $p_c$, the density of holes within the small-sized black clusters is negligible; hence $\chi(p)$ is positive and increases with increasing $p$. On the other hand, for $p > p_c$, and $1 - p \ll 1$,
there is a single infinite black cluster with finite (white) holes and thus $\chi(p) < 0$, in accordance with equation (3). In the intermediate range of $p$, which includes $p_c$, the MEC decreases as the black clusters grow in size and merge to generate a single infinite component as $p$ passes the percolation threshold at $p_c$. We see that the typical features of the MEC are governed by the interplay of the complementary finite black and white clusters. The percolation transition with the singular emergence of an infinite cluster leaves its signature only in the zero crossing of $\chi(p)$ at $0 < p_0 < 1$ with a value of $p_0$ expected to be comparable with $p_c$.

2. Percolation thresholds and the zero crossing of the MEC

The idea that the zero crossing of the MEC should occur near the critical probability $p_c$ is plausible and is supported, for instance, by the fact that $p_0 = p_c = 1/2$ for site percolation on the self-matching triangular lattice, but it calls for a more precise and quantitative argument. Here we will first compare $p_0$ with $p_c$ and we shall find that $p_0$ provides generally a tight upper bound to $p_c$ whenever $p_c > 1/2$.

2.1. Archimedean lattices

To begin with, we consider the 11 Archimedean lattices, where all vertices are equivalent up to a symmetry operation and all faces are regular polygons. The most prominent members of this class are the triangular, the square, the honeycomb and the kagomé lattice. Each lattice is uniquely characterized by the number of edges $n_i$ of the polygons surrounding a vertex [17]. A lattice of coordination number $z$ is therefore conveniently denoted by the symbols $(n_1, \ldots, n_z)$, where $a_i$ identical consecutive polygons are often abbreviated as $n_i^{a_i}$. For example, a vertex of the square lattice is surrounded by four squares. The vertex type of the square lattice is therefore $(4, 4, 4, 4)$ or $(4^4)$ in the abbreviated notation. Similarly, a vertex of the kagomé lattice is surrounded by alternating triangles and hexagons and has vertex type $(3, 6, 3, 6)$. With this notation, the MECs of the Archimedean lattices are given by

\[ \chi(p) = p(1 - p) \left( 1 - p \sum_{i=1}^{z} \frac{1}{n_i} \sum_{\mu=0}^{n_i-3} p^{\mu} \right). \]
Figure 3. The percolation threshold $p_c$ is slightly below the zero crossing $p_0$ of the MEC whenever $p_c > \frac{1}{2}$. This order is reversed, if $p_c < \frac{1}{2}$, as is apparent in the panel on bond percolation. The solution $p^*$ of equation (17) provides a very accurate estimate of $p_c$. The deviation $|p_c - p^*|$ exceeds 0.01 only for very open lattices with high percolation thresholds. Lattices are in the order of decreasing percolation threshold. For vertex configurations, numerical values of $p_c$ and $p^*$ for the 2-uniform lattices; see table 4 in the supplementary material. Numerical estimates of $p_c^{\text{site}}$ for the Archimedean lattices are taken from [14]; values for $p_c^{\text{bond}}$ are from [15,16].

The percolation thresholds of Archimedean lattices are known to very high precision [14]. In figure 3, we compare $p_c$ to the zero crossing $p_0$ of $\chi(p)$. For the self-matching triangular lattice $p_0 = p_c = \frac{1}{2}$. Furthermore, a close relation appears to exist between $p_c$ and $p_0$ even for lattices with $p_c > \frac{1}{2}$: $p_c$ is bounded from above by $p_0$, with $p_0 - p_c$ increasing steadily with $p_c - \frac{1}{2}$. Similar observations can be made for the duals of the Archimedean lattices, see figure 2 of the supplementary material.

2.2. 2-uniform lattices

Next, we study the larger class of 2-uniform lattices, which again consist of regular polygons but have two distinct vertex types [17]. The two vertex types can occur with different abundances, and a 2-uniform lattice is commonly denoted by $s_1(n_1^1, \ldots, n_z^1) + s_2(n_1^2, \ldots, n_z^2)$, where $s_i$ is the fraction of vertices that are of type $i$. The MECs are given by the straightforward generalization of equation (6)

$$\chi(p) = p(1-p) \left( 1 - p \sum_{\nu=1,2} \sum_{i=1}^{s_\nu} \frac{n_\nu^i}{n_\nu^i} \sum_{\mu=0}^{n_\nu^i-3} p^\mu \right),$$

where $n_\nu^i$ is the number of $i$-gons of type $\nu$ and $s_\nu$ is the fraction of vertices of type $\nu$.
which can obviously be generalized to any finite number of vertex types. We are not aware that the percolation thresholds of 2-uniform lattices have been previously determined, and we therefore estimated them using an algorithm adopted from [18]. Again, \( p_0 \) provides a tight upper bound to \( p_c \) as shown in figure 3. The vertex configurations, as well as \( p_0 \) and the estimate of \( p_c \) for the 2-uniform lattices are given in table 4 of the supplementary material.

2.3. Bond percolation in two dimensions

Every bond percolation problem is equivalent to site percolation on the covering lattice. The covering lattices, however, are not necessarily planar but decorated mosaics. A decorated mosaic is constructed from a planar lattice, where in a subset of the faces all diagonal connection have been added (the face is decorated). A pair of lattices where complementary sets of faces are decorated constitutes a pair of matching lattices in the sense of equation (1) [13]. Calculating the MEC of decorated mosaics is slightly more laborious, but a general framework for the calculation has been presented in [19]. Using this framework, we calculated the MEC of the covering lattices of all Archimedean lattices with vertices \((n_1,\ldots,n_z)\):

\[
\chi(p) = -p + \frac{2}{z} (1 - (1 - p)^z) + \sum_{i} \frac{2}{z n_i} p^{n_i}. \tag{8}
\]

Comparing numerical estimates of \( p_c \) [15, 16] to \( p_0 \) confirms \( p_0 > p_c \) if \( p_c > \frac{1}{2} \) (figure 3), albeit with one notable exception for lattice 6 with vertex configuration \((3,4,6,4)\). For lattices with \( p_c < \frac{1}{2} \) the order of \( p_c \) and \( p_0 \) is reversed, as expected from the matching properties of \( p_c \) and \( \chi(p) \).

The relation between \( p_c \) and \( p_0 \) is not restricted to regular lattices but also holds for the quasi-periodic Penrose tiling and random tessellations of the plane such as Voronoi and Delauny tessellations; see the supplementary material for values of \( p_c \) and \( p_0 \) and the polynomials of the MECs.

2.4. Randomly decorated mosaics

Instead of regular decorated mosaics, we now consider lattices where each face is decorated with probability \( p_{\text{dec}} \), as illustrated in figure 4(a). We are not aware that this type of percolation process, which bears some similarity to a bond-site percolation processes, has been studied before. Our numerical estimates of percolation thresholds of a randomly decorated mosaic decrease smoothly from \( p_c(p_{\text{dec}} = 0) \) to \( p_c(p_{\text{dec}} = 1) \), in accord with the containment property [20]. Randomly decorated lattices fulfill the statistical matching property \( p_c(p_{\text{dec}}) + p_c(1 - p_{\text{dec}}) = 1 \), from which \( p_c(0.5) = 0.5 \) follows. The averaging over the different decoration states of the lattice is straightforward and the MEC of randomly decorated mosaics can be calculated in the same way as that of regular decorated mosaics. For the hexagonal lattice one finds

\[
\chi(p, p_{\text{dec}}) = (1 - p_{\text{dec}}) \chi_{\text{hex}}(p) + p_{\text{dec}} \tilde{\chi}_{\text{hex}}(p). \tag{9}
\]

From equation (2) follows the symmetry relation \( \chi(p, p_{\text{dec}}) = -\chi(1 - p, 1 - p_{\text{dec}}) \). Hence, we have \( p_0(p_{\text{dec}}) + p_0(1 - p_{\text{dec}}) = 1 \) in analogy to \( p_c(p_{\text{dec}}) + p_c(1 - p_{\text{dec}}) = 1 \). Our results
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Figure 4. (a) A lattice face is decorated, when all diagonal connections across the faces have been added to the lattice graph, as illustrated here for three faces of the hexagonal lattice. We consider randomly decorated lattices where each face is decorated with probability $p_{\text{dec}}$. (b) The site percolation threshold $p_c$ decreases smoothly as the degree of decoration is varied from $p_{\text{dec}} = 0$ to 1. The zero crossing $p_0(p_{\text{dec}})$ of $\chi(p, p_{\text{dec}})$ provides a tight upper bound to $p_c(p_{\text{dec}})$ if $p_c(p_{\text{dec}}) > \frac{1}{2}$ and vice versa. The solution of equation (17), $p^*(p_{\text{dec}})$, lies within 0.005 of $p_c(p_{\text{dec}})$ with the largest deviations at full or no decoration.

for the randomly decorated hexagonal lattice are shown in figure 4(b). The zero crossing $p_0(p_{\text{dec}})$ follows $p_c(p_{\text{dec}})$ very closely, being a tight upper bound for $p_{\text{dec}} > \frac{1}{2}$ and a lower bound otherwise. Similar results can be obtained for other Archimedean lattices (data not shown).

3. The EC of critical percolation and estimation of $p_c(\Lambda)$

In the previous sections, we saw that $p_c(\Lambda)$—a global property of the lattice—is followed rather closely by $p_0(\Lambda)$, a locally computable quantity. Here, we are going to explore the relation of $p_c(\Lambda)$ with $p_0(\Lambda)$ in more detail by evoking a generally accepted scaling form for the densities $n_s(p)$ of large clusters at $p_c$ [21]. These densities determine $\chi(p)$ according to equation (2). Moreover, they also enter in the sum rules [4]

$$p = \sum_s s n_s(p) + \bar{P}_\infty(p), \quad \bar{p} = \sum_s s \bar{n}_s(\bar{p}) + \bar{P}_\infty(\bar{p}),$$

which express the probability for a particular vertex to be black ($p$) or white ($\bar{p}$).

In 2D lattice graphs only a single critical point exists, so that $P_\infty(p_c) = 0 = \bar{P}_\infty(\bar{p}_c)$. At the threshold the scaling ansatz reads

$$n_s(p_c) \simeq a(\Lambda) s^{-\tau} \quad \text{and} \quad \bar{n}_s(\bar{p}_c) \simeq \bar{a}(\bar{\Lambda}) s^{-\tau}. \quad (10)$$

The non-universal amplitudes $a(\Lambda)$ and $\bar{a}(\bar{\Lambda})$ account for the particular structure of the underlying lattice and its matching partner, whereas the value of the universal exponent $\tau = 187/91$ is known exactly in two dimensions [4, 22, 23].

In order to exploit the scaling hypothesis, we define

$$\chi_{s_0}(p) := \chi(p) - \sum_{s=1}^{s_0} [n_s(p) - \bar{n}_s(\bar{p})], \quad (11)$$

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and set

$$\chi_{s_0}(p_c) \simeq (a - \bar{a}) \sum_{s>s_0} s^{-\tau}. \quad (12)$$

Likewise,

$$\Delta_{s_0}(p) := (p - \bar{p}) - \sum_{s=1}^{s_0} s \left[ n_s(p) - \bar{n}_s(\bar{p}) \right]; \quad (13)$$

$$\Delta_{s_0}(p_c) \simeq (a - \bar{a}) \sum_{s>s_0} s^{1-\tau}. \quad (14)$$

After elimination of the non-universal scaling amplitudes, we arrive at

$$\chi_{s_0}(p_c) \simeq \frac{\zeta(\tau, s_0)}{\zeta(\tau - 1, s_0)} \Delta_{s_0}(p_c), \quad (15)$$

where $\zeta(\tau, s_0) = \sum_{s=1}^{\infty} (s + s_0)^{-\tau}$ is the Riemann zeta function with offset $s_0$.

The relation (15) may be applied as an equality, for instance, (i) to determine a value of $s_0$ from the requirement that the left- and right-hand sides equalize within a prescribed accuracy, or (ii) to estimate $p_c(\Lambda)$. For the latter purpose, we rewrite equation (15) by substituting the defining expressions (12) and (14) for $\chi_{s_0}(p)$ and $\Delta_{s_0}(p)$. The result is

$$\chi(p) = \frac{\zeta(\tau, s_0)}{\zeta(\tau - 1, s_0)} \left[ (2p - 1) - \sum_{s=1}^{s_0} s \left[ n_s(p) - \bar{n}_s(\bar{p}) \right] \right] + \sum_{s=1}^{s_0} \left[ n_s(p) - \bar{n}_s(\bar{p}) \right]. \quad (16)$$

The real root, $\hat{p}(s_0)$, $0 < \hat{p}(s_0) < 1$, of this polynomial equation provides an estimate for $p_c$, the accuracy of which increases with $s_0$. For the square lattice, the cluster numbers $g_{st}$ and $\bar{g}_{st}$ are known up to $s = 12$ [24] and we calculated $\hat{p}(s_0)$ for $s_0 = 0, \ldots, 12$. Figure 5 shows how $\hat{p}(s_0)$ approaches $p_c$ with increasing $s_0$. The zeta functions $\zeta(\tau, s_0)$ and $\zeta(\tau - 1, s_0)$ can be approximated by integrals and their ratio evaluates to $(\tau - 2)(\tau - 1)^{-1}(s_0 + 1)^{-1}$. In many cases corrections for small clusters are not even necessary, and using $s_0 = 0$ and

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Figure 5. Site percolation on the square lattice: the solution $\hat{p}(s_0)$ of equation (16) approaches $p_c$ with increasing $s_0$. 
Table 1. The deviation of the estimate \( \hat{p}(s_0, \Lambda) \) from \( p_c(\Lambda) \) decreases rapidly when \( s_0 \) is increased from zero to two.

| \( s_0 \) | \( 6^3 \) | \( 4, 8^2 \) | \( 4, 6, 12 \) | \( 3, 12^2 \) | \( \frac{1}{2}(3, 4, 3, 12^2) \) |
|---|---|---|---|---|---|
| 0 | -0.01027 | -0.02258 | -0.03184 | -0.04543 | -0.05085 |
| 1 | -0.00553 | -0.00901 | -0.01530 | -0.01240 | -0.02093 |
| 2 | -0.00551 | -0.00283 | -0.00701 | -0.00615 | -0.00937 |

The approximation for the zeta function yields the simple equation

\[
\chi(p) = \frac{\tau - 2}{\tau - 1}(2p - 1),
\]

with a unique solution \( p^* \), \( 0 < p^* < 1 \). For all lattices discussed so far, \( p^* \) is a fairly accurate estimate of \( p_c \), as shown in the figures 3 and 4.\(^4\) Further examples may be found in the supplementary note. Among the lattices studied here, the deviation of \( p^* \) from \( p_c \) was greatest for the lattices with very high percolation thresholds (compare figure 3) which are inhomogeneous on small scales. To test whether these deviations are caused by the smallest clusters and holes, we enumerated the clusters and holes of size one and two for the hexagonal lattice, the \( (4, 8^2) \) lattice, the \( (4, 6, 12) \) lattice, the \( (3, 12^2) \) lattice, and the 2-uniform lattice with vertex configuration \( 1^2(3, 4, 3, 12) + 1^2(3, 12^2) \). The deviation of \( \hat{p}(s_0) \) from \( p_c \) decreases when the contributions of the smallest clusters and holes are subtracted, i.e. \( s_0 \) is increased from 0 to 2; see table 1.

The estimation of the threshold value \( p_c \) via equation (17) will fail, if small clusters or small holes are much more abundant at the critical point than an extrapolation of the asymptotic law for large clusters would suggest. In particular, this is obvious for lattices that contain a substructure which does not contribute to large scale connectivity but dominates the density of small clusters.

4. Three-dimensional lattices

The combinatorial EC of percolation patterns \( P \) on a \( d \)-dimensional lattice is given by the alternating sum of the numbers of \( k \)-dimensional lattice cells, \( k = 0, \ldots, d \), contained in \( P \). Thus, in the case \( d = 3 \), equation (4) is replaced by

\[
\mathcal{X}(P) = \#v - \#e + \#f - \#c,
\]

where \( \#c \) is the number of black three-dimensional polyhedral lattice cells. The resulting MEC of black clusters in the case of site percolation on a simple cubic (sc) lattice, for example, is given by

\[
\chi_{sc}(p) = p - 3p^2 + 3p^4 - p^8.
\]

The black vertices are connected, i.e. they are part of the same cluster, if they are joined by a path of black nearest neighbors on the lattice. As in the two-dimensional case, the black clusters partition the white vertices into an aggregate of clusters with a complementary

\(^4\) In many cases, the integral approximation of the zeta function yields better results than the exact ratio, which is probably due to a subtle cancelation of errors.
Figure 6. The graphs of the MEC of the simple cubic (sc) and body-centered cubic (bcc) lattice. The bcc lattice has the same black and white connectivities and is hence invariant to the substitution $p = 1 - p$.

connectivity, such that there is a one-to-one correspondence between cavities in black clusters and finite white clusters, as well as between the cavities in white clusters and finite black clusters. A white vertex of the simple cubic lattice, for example, is connected to all 26 vertices on the boundary of the eight surrounding lattice cubes, in contrast to the six neighbors of the black vertices, which correspond to lattice bonds. In addition to cavities, black clusters can have handles, i.e. they can be homeomorphic to a solid torus or objects of higher genus. Each handle of a black cluster is pierced by precisely one handle of a white cluster. From these duality relations and the 3D analogue of equation (3)

$$X(P) = \# \text{clusters} - \# \text{handles} + \# \text{cavities},$$

we see that EC of white clusters is identical to that of black clusters. Hence, the MEC of white clusters is $\chi(\bar{p}) = \chi(1 - \bar{p})$ with $\bar{p} = 1 - p$.

The graph of $\chi_{sc}(p)$ shown in figure 6 is typical for the MECs in $d = 3$, where the MECs have two distinct non-trivial zero crossings $p_{bc}^b$ and $1 - p_{bc}^w$. In the intermediate regime where $\chi(p) < 0$, the MEC is dominated by interwoven white and black handles. The percolation thresholds of the lattice with black $p_{bc}^b$ and white $p_{bc}^w$ connectivity are different in general. In the range $p_{bc}^b < p < 1 - p_{bc}^w$ a single infinite black cluster coexists with a single infinite white cluster. In order to check for a possible link between zero crossings of $\chi(p)$ and thresholds, we compare in table 2 $p_{bc}^b$ and $p_{bc}^w$ with simulation values $p_{sc}^b$ and $p_{sc}^w$ for the sc lattice, face-centered cubic (fcc) lattice and the body-centered cubic (bcc) lattice. The calculation of the MECs for fcc and bcc lattices is reported in the supplementary note. As figure 6 already indicates, $p_{bc}^b$ and $p_{bc}^w$ are both upper bounds for $p_{sc}^b$ and $p_{sc}^w$, and they are becoming tighter as the (effective) coordination numbers increase.

The task to devise a threshold estimator based on the above findings appears to be more difficult than in the two-dimensional case, and it is left for future work.

5. Continuum percolation

So far, we have dealt with the EC of percolating clusters on geometric lattices. Let us finally make a few remarks to indicate that the features of the EC induced by the percolation thresholds persist in the case of continuum percolation. Consider the standard Boolean model where penetrable convex grains are positioned randomly at
Table 2. Numerical values for $p_0$ and $p_c$ of the cubic lattices for black and white connectivities. The bcc lattice has equal black and white connectivities.

| Lattice | $z$ | $p_0$  | $p_c$ |
|---------|-----|--------|-------|
| sc (black) | 6  | 0.3940 | 0.3116 |
| fcc (black) | 12 | 0.2370 | 0.1992 |
| bcc | 14 | 0.2113 | 0.175 |
| fcc (white) | 18 | 0.1616 | 0.136 |
| sc (white) | 26 | 0.1139 | 0.097 |

$^a$ Threshold densities are taken from [25].
$^b$ Threshold densities are taken from [26].

Poisson distributed points in $\mathbb{R}^d$. The grains may be multidispersed, having random size, shape and orientation. By using results from integral geometry, the MEC of patterns formed by clusters of overlapping grains can be calculated exactly [27]. In $d = 2$ the MEC reads

$$\chi_2(\eta) = \eta(I - \eta)e^{-\eta}, \quad \eta = \rho a,$$

with the grain density $\rho$, and the dimensionless ratio $I = u/4\pi a$; $a$ and $u$ denote the average grain area and perimeter, both assumed to be distributed independently from the grain locations. In the case of monodispersed convex grains, $I \geq 1$ is an isoperimetric ratio. For $d = 3$ one finds

$$\chi_3(\zeta) = \left(1 - 3I_1\zeta + \frac{3\pi^2}{32}I_2\zeta^2\right)e^{-\zeta}, \quad \zeta = \rho v.$$

Here, $I_1 = sb/6v$, $I_2 = s^3/36\pi v^2$; $b$, $s$ and $v$ are the averages of the grain mean breadth, surface area and volume, respectively. Again, for monodispersed convex grains, $I_1 \geq 1$, $I_2 \geq 1$. The graphs of $\chi(p)$ and $\bar{\chi}(p)$, when plotted as functions of the mean coverage $0 \leq 1 - e^{-\eta} < 1$ and $0 \leq 1 - e^{-\zeta} < 1$, are similar to the graphs of the corresponding lattice MECs: $\chi_2(\eta)$ has a single zero at $\eta_0 = I^{-1}$, $\chi_3(\zeta)$ has two zeros located at $\zeta_0 = (96/\pi)(bv/s^2)(1 - \sqrt{1 - (\pi/24)(s/b^2)})$. For monodispersed discs $\eta_0 = 1$, which may be compared with the threshold value $\eta_c \approx 1.12$. Monodispersed spheres yield $\zeta_0^- = 0.377$, to be compared with the percolation threshold of penetrable spheres, $\zeta_c \approx 0.34$ [28]. The interpretation of the continuum MECs in terms of cluster structures can be carried over unchanged from the lattice examples. Thus, for instance, $\zeta_0^+$ is expected to provide a quick estimate for the percolation threshold $\zeta_0^+$ of the void space defined as the set complement of the pattern by the clusters of overlapping grains.

6. Summary and discussion

Taken together, the equations (16) and (17) represent our main result. The relation (17) connects the universal scaling behaviour of percolating clusters at $p_c$ with their specific topological structure, as expressed by the mean Euler characteristic. It provides a novel and parameter-free estimate of threshold values for two-dimensional lattices, which is remarkably accurate. In the case of self-matching lattices equation (17) reproduces the exact values $p_c = 1/2$, and offers an explanation for the numerical finding that the zero
crossing of the MEC, $p_0$, is a tight upper (lower) bound for the threshold $p_c$ if $p_c > 1/2$ ($p_c < 1/2$).

Over the years, a variety of ‘universal’ approximate formulae for predicting percolation thresholds have been devised [14], [29]–[31]. Most of these proposals fit an empirical relation with a number of free parameters to a set of known thresholds. Recently, Wierman and Naor [32] introduced a list of criteria for the evaluation of such formulae. Accordingly, these should (1) be well defined, (2) be easily computable, (3) provide values only between 0 and 1, (4) depend only on the adjacency structure of the lattice, (5) be accurate, (6) be consistent with the matching relationship, and (7) be consistent with the containment principle.

Equation (17) complies with the first six of these requirements, as can be inferred from its deduction and from the comparison of our estimates with precise numerical threshold values. We have not checked in detail criterion (7). The claim that our $p_c$-estimation is well defined may perhaps be questioned, since equation (17) involves an extrapolation of the scaling ansatz to the smallest cluster sizes. However, this ad hoc simplification can be removed by going back to the ‘master equation’ (16), which provides means to systematically correct for small-scale irregularities, as shown in table 1.

We mentioned the exact expressions of the mean Euler characteristic for 3D cubic lattices and for the Boolean model of continuum percolation in two and three dimensions. The close linking of the zero crossings of these MECs to the respective threshold densities appears to persist and underlines once more the role of the Euler characteristic as the appropriate concept for describing the topological aspects of percolation. But to apply this intriguing fact for the construction of threshold estimators for three dimensions and for continuum models remains a challenging problem.

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