Site percolation thresholds for Archimedean lattices

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Precise thresholds for site percolation on eight Archimedean lattices are determined by the hull-walk gradient-percolation simulation method, with the results $p_c = 0.697043$, honeycomb or (6^3) , 0.807904 $(3,12^2)$, 0.747806 (4,6,12), 0.729724 $(4,8^2)$, 0.579498 $(3^4,6)$, 0.621819 (3,4,6,4), 0.550213 $(3^3,4^2)$, and 0.550806 $(3^2,4,3,4)$, with errors of about $\pm 3 \times 10^{-6}$. [The remaining Archimedean lattices are the square (4^4) , triangular (3^6) , and Kagomé (3,6,3,6), for which p_c is already known exactly or to a high degree of accuracy.] The numerical result for the $(3,12^2)$ lattice is consistent with the exact value $[1-2\sin(\pi/18)]^{1/2}$. The values of p_c for all 11 Archimedean lattices, as well as a number of nonuniform lattices, are found to be well correlated by a nearly linear function of a generalized Scher-Zallen filling factor. This correlation is much more accurate than recently proposed correlations based solely upon coordination number. [S1063-651X(99)11207-8]

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I. INTRODUCTION

The Archimedean tilings were first elucidated and published by Kepler (a translation of which can be found in Ref. [1]). These tilings received their name from references in Kepler's paper to Archimedes' descriptions of regular solid polyhedra, which are related to these two-dimensional (2D) lattices. The significance of the Archimedean tilings or lattices, which are shown in Fig. 1, is that they are the complete set of lattices having infinite tessellation in which all vertices are equivalent. This property has made them useful in the study of mathematics [2], crystallization [3,4], and statistical mechanics [5], as well as percolation [6]. The familiar square, triangular, honeycomb, and Kagomé lattices are all Archimedean, the first three being the regular lattices. The Archimedean lattices are also called *uniform* lattices.

The primary goal of this study was to determine precise numerical values of the site percolation threshold p_c for all Archimedean lattices for which accurate values were not previously known. A few years ago, d'Iribarne, Rasigni, and Rasigni determined p_c for all but one of the Archimedean lattices to about three significant figures [6], using a method based upon the analysis of the minimum spanning tree of clusters [7]. More recently van der Marck [8,9] determined the thresholds for three of these lattices to nearly four figures. The threshold for the honeycomb lattice-a commonly used lattice for percolation studies-was previously also known to about four figures [9-11]. Here we extend the precision of these thresholds to nearly six significant figures, using the gradient-percolation method [12,13] simulated by the hull-walk algorithm [14]. We did not consider square, triangular, and Kagomé lattices, as p_c (site) for these cases is either known exactly (triangular and Kagomé [15]), or has already been measured to a high degree of precision (square [16]).

The second goal of this study was to explore the dependence of p_c upon lattice characteristics and to determine to

what extent an accurate correlation formula can be found for these and other 2D lattices. Recently Galam and Mauger (GM) proposed "universal" formulas for percolation thresholds [17–21]; these formulas have also been discussed at length by van der Marck [8,9,22–24]. Archimedean lattices provide an excellent resource for studying such formulas, because these lattices possess a range of coordination numbers from 3 to 6 and a variety of other lattice characteristics. We find a fairly good correlation based upon certain topological characteristics of the lattice, and demonstrate its accuracy when applied to a number of additional (nonuniform) 2D lattices where p_c has been previously measured.

Nomenclature

Neither Kepler, Archimedes, nor anyone else to our knowledge assigned common names to all the Archimedean



FIG. 1. The 11 Archimedean lattices, in which all vertices are equivalent. Lattices are designated using the notation of Grünbaum and Shephard [23], as explained in the text.

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TABLE I. New values of p_c determined here for site percolation on the Archimedian lattices. Lattice nicknames in quotes are our own. N is the total random numbers generated.

Lattice	Measured p_c	Ν	Previous values
(3,12 ²) "star"	0.807 904(4)	4.1×10^{11}	0.807 900 764 (exact)
(4,6,12) "cross"	0.747 806(4)	2.6×10^{11}	0.746 [6]
(4,8 ²) "Briarwood"	0.729 724(3)	2.6×10^{11}	0.729 [6], 0.7298(1) [8,41]
(6 ³) honeycomb	0.697 043(3)	4.0×10^{11}	0.6973(8) [10], 0.6962(6) [11], 0.6971(2) [9]
(3,4,6,4) "bounce"	0.621 819(3)	2.9×10^{11}	0.620 [6]
(3 ⁴ ,6) "bridge"	0.579 498(3)	2.9×10^{11}	$0.55 \le p_c \le 0.6$ [34]
(3 ² ,4,3,4) "puzzle"	0.550 806(3)	2.8×10^{11}	0.550 [6]
(3 ³ ,4 ²) "direct"	0.550 213(3)	2.9×10^{11}	0.549 [6], 0.5504(2) [8,41]

lattices. Grünbaum and Shephard [25] use a general notation to categorize such lattices in terms of the set of polygons which surround each vertex, $(n_1^{a_1}, n_2^{a_2}, ...)$. Going clockwise around a vertex, the numbers n_i denote the number of sides of each polygon, and the superscript a_i refers to the number of these polygons adjacent to each other. For example, the triangular lattice has six triangles around a given point, and is designated (3⁶). The labels for all the Archimedean lattices are shown in Fig. 1.

For convenience in our work we did assign nicknames to the lattices, which are listed in Table I. The (4,6,12) lattice is called the "cross" lattice because of the cross in Fig. 3; the $(4,8^2)$ lattice is named after our local shopping mall, Briarwood, which like many such malls has tiles of this shape on its floor; the $(3^3,4^2)$ lattice is called the "direct" lattice because of its directed structure, etc. The origins of the rest of the names are, we hope, somewhat more obvious. Note that the $(3,12^2)$ lattice has been called the "3-12" lattice in the literature, and the $(4,8^2)$ lattice has been called the "bathroom tile" lattice.

II. METHOD

A. Hull-gradient walk

To find p_c we employ the hull-gradient method [26], which we previously used to determine p_c for site percolation on the square lattice [27] and for bond percolation on the Kagomé lattice [28] to more than six significant digits of precision. This method is more efficient than the traditional crossing-probability method (e.g., Ref. [29]), with an error near the statistical limit,

$$\sqrt{\langle (\Delta p_c)^2 \rangle} = \sqrt{\frac{p_c(1-p_c)}{N}}$$
(1)

where *N* is the total number of random numbers generated. In Ref. [26] we verified the hull-gradient method for site percolation on the Kagomé lattice, whose threshold is known exactly. Here we provide an additional confirmation of the method using the $(3,12^2)$ lattice, whose site threshold we also find exactly. Note that the triangular lattice does not provide a useful test of the hull-gradient method, because by simple symmetry it gives the exact result $p_c = \frac{1}{2}$ within statistical error for any gradient.

In gradient percolation [12,13], a linear gradient of occupied sites is applied in the vertical direction of the lattice. As the height increases, the concentration of occupied sites also increases. This gradient forms two "land masses" within the lattice: a continuous region of occupied sites located at the top of the lattice, and a continuous region of vacant sites located at the bottom (Fig. 2). The boundary between these two regions forms a path whose average height provides an estimate for p_c .

To make this method efficient for finding p_c , a hullgenerating walk [14,30], which simultaneously generates and identifies the interfacial boundary, is employed [26]. The status of a site encountered by the walk, whether occupied or vacant, is determined by generating a random number and comparing that number with the occupation probability for that height. If the walk does not arrive at a given site, the status of that site will not be determined, and no random number will be generated for it. We believe that the hullgradient method is the most efficient way to determine p_c for 2D lattices; it is also simple to program, as it involves no lists or cluster labeling algorithms.

For each gradient $|\nabla p|$, an estimate of p_c may be obtained by taking the ratio of occupied to total (occupied plus vacant) perimeter sites belonging to the hull [13]:

$$p_c(|\nabla p|) = \frac{n_{\rm occ}}{n_{\rm occ} + n_{\rm vac}}.$$
(2)

As the size of the system is increased or the gradient is decreased, $p_c(|\nabla p|)$ approaches p_c linearly in $|\nabla p|$. Thus a simple extrapolation of the data for finite gradients gives the infinite-system value. In practice, we considered gradients sufficiently small [typically of the order of $10^{-4} \Delta p/(\text{lattice spacing})$] so that the extrapolation from the final point to



FIG. 2. The hull-generating walk along a percolation gradient for the honeycomb lattice. Filled circles denote occupied sites, and heavy lines show the hull of the percolating region. The arrow points to the starting point of the walk.



FIG. 3. The Archimedean lattices transformed to a square array, for use in the computer simulation. Some lattices were distorted in the vertical direction, but in all cases the actual lattice height, rather than the height in the square array, was used to determine the site occupation probability.

zero gradient was of the order of the error bars of that last point. Additional details of the method were given in Refs. [26, 28].

B. Computer techniques

In the simulation, the status of all points visited by the walk must be stored in computer memory. To accomplish this efficiently, all of the Archimedean lattices were transformed to align on rectilinear grids, as shown in Fig. 3. Note that the gradient was not applied directly to these squared-off forms, as some lattices had to be distorted in the vertical direction. Instead, all numerical calculations were performed so that the height of the point in the original, undistorted, lattice was used to find p(z). Previously we showed (for bond percolation on the Kagomé lattice) that assigning p(z) this way yields the best linear scaling of p_c vs gradient [28]. For two lattices, we considered two different orientations of the lattice and found similar results, as discussed in the Appendix.

The lattices were initialized by filling the top half of the first column with occupied sites and the lower half with vacant sites, in order to prevent the walk from closing on itself at the start of a run (Fig. 2). Periodic boundary conditions were applied in the horizontal direction, and each new column to the right was cleared as it was first visited, allowing the simulation to run indefinitely and have no boundary effects from the horizontal ends of the system. The maximum distance the walk traveled horizontally from the front was tracked to detect if wraparound errors occurred; if they did, the system size and/or gradient was adjusted accordingly, and the run was restarted with the expanded system.

Random numbers were generated using the shift-register sequence generator R7(9689) [31,32] defined by

$$x_n = x_{n-471} \,^{\wedge} x_{n-1586} \,^{\wedge} x_{n-6988} \,^{\wedge} x_{n-9689}, \tag{3}$$

where $\hat{}$ is the bitwise exclusive-or operation. This "fourtap" generator is equivalent to decimating by 7 (taking every seventh term) of the sequence generated by the two-tap rule R(9689) ($x_n = x_{n-471} \hat{} x_{n-9689}$) given by Zierler [33], where the decimation has the effect of greatly reducing the three-



FIG. 4. Percolation threshold vs lattice gradient for the $(3,12^2)$ lattice. As the gradient becomes smaller, the lattice approaches infinite size. The percolation threshold can be estimated from the *y* intercept of a linear regression of results from finite lattices.

and four-point correlations of the two-tap generator [31]. Our previous work has shown that this generator does not appear to introduce errors in simulations of this kind [26,28].

III. RESULTS AND DISCUSSION

A. Percolation thresholds

For each lattice, p_c was plotted as a function of the gradient. Figure 4 shows a representative plot for the $(3,12^2)$ lattice. In all cases, a linear relationship was observed between the magnitude of the gradient and the estimate $p_c(|\nabla p|)$, as found previously for the square [13] and Kagomé lattices [28]. The value at the intercept of the y axis represents p_c for an infinite lattice (zero gradient), and these values are reported in Table I. Also shown in Table I for each lattice is the quantity of random numbers generated, which is identical to the total number of occupied and vacant hull sites, because one random number is generated for each new site visited. These simulations consumed a total of several months of computer time on Sun and HP workstations.

For all our values, the statistical error is about 3×10^{-6} , as determined using Eq. (1), multiplied by a factor of about 1.5 which we found in other studies to be approximately appropriate for the minimum gradients used here. Our results are seen to be consistent with previous works.

For the $(3^4,6)$ lattice, p_c has never been previously measured, to our knowledge. However, Préa [34] recently conjectured that its value lies within the interval [0.55, 0.6], based upon a study of the distance sequences c_n , defined as the number of sites n steps (chemical distance) from the origin. For the Archimedean lattices Préa found a monotonic relation between p_c (site) using d'Iribarne, Rasigni, and Rasigni's measurements, and $c \equiv \lim_{n\to\infty} \inf(c_n/n)$ (although three different lattices with different p_c —the square, Kagomé, and (3,4,6,4)—share the same value c=4), and conjectured that the $(3^4,6)$ lattice fits into this ordering, implying the above bounds. This conjecture is confirmed by our result $p_c = 0.579\,498(3)$.

B. Exact percolation threshold for the $(3,12^2)$ lattice

The exact threshold for the $(3,12^2)$ lattice can be derived by a simple argument. Although we found this result inde-



FIG. 5. Derivation of the exact percolation threshold for the $(3,12^2)$ lattice. Replacing the dashed bonds with single points leads to the Kagomé lattice.

pendently, we have since learned that Whittington also derived it (unpublished), as quoted in print recently by Guttmann [35]. Our proof is based upon the similarity of structure between this lattice and the Kagomé lattice. In Fig. 5, the $(3,12^2)$ lattice is shown with the triangle bonds in bold and the bonds between the triangles as dashed lines. If the dashed lines are reduced in length, the $(3,12^2)$ lattice transforms into the Kagomé lattice. Similarly, the sites on both ends of the dashed line in the $(3,12^2)$ lattice (marked by the large circle in the figure), taken together, are equivalent to a single point on the Kagomé lattice.

Let *p* be the probability that a given site on the $(3,12^2)$ lattice is occupied. Then p^2 is the probability that both sites at the ends of the dashed bonds in Fig. 5 are occupied, which is the only case that the bond will permit flow. Now, replacing that dashed bond by a single site, occupied only if both of the original sites were occupied, the $(3,12^2)$ lattice becomes the Kagomé lattice. Whatever paths of connected sites existed on the $(3,12^2)$ lattice remain on the Kagomé lattice. Therefore if the $(3,12^2)$ lattice is at the criticality, so is the Kagomé lattice. At the percolation threshold, p_c on the Kagomé lattice is $1-2\sin(\pi/18)$. Therefore, for the $(3,12^2)$ lattice,

$$p_c = [1 - 2\sin(\pi/18)]^{1/2} = 0.807\,900\,764\dots$$
 (4)

Our numerical estimate 0.807 904(4) is consistent with this result, providing a further confirmation of the gradient percolation method and our error analysis.

An essential point in the above argument is that the polygons are triangles, so that when a pair of occupied-vacant points on the $(3,12^2)$ lattice is replaced by a single vacant site on the Kagomé lattice, the removal of that occupied site does not affect percolating paths on the other two sites of the triangle. One cannot apply this argument to relate p_c of the $(4,8^2)$ lattice to that of the square lattice, for example, because there the central polygons are squares, and the removal of an occupied site from one corner of a square affects percolating paths through other vertices.

C. Galam and Mauger's universal formula for p_c

Early in the work of percolation, thresholds were related with coordination number q using relatively simple formu-



FIG. 6. Thresholds plotted as $\ln 1/p_c$ vs $\ln(q-1)$. (•) regular lattices (from left to right: honeycomb, square, and triangular lattices), (\Box) Kagomé, (Δ) less-common Archimedean lattices, (\times) nonuniform lattices. Dashed line: GM's class 1 formula; solid line, GM's class 2 formula.

las, such as $p_c \propto 1/(q-1)$. More recently, GM [20,21] expanded upon this idea and proposed a "universal" formula given by

$$p_c = p_0 [(d-1)(q-1)]^{-a} d^b,$$
(5)

where *d* is the dimensionality, and the constants *a*, p_0 , and *b* depend upon the class and percolation type, with b=a for bond percolation and b=0 for site percolation. They divided percolation systems into two different classes, each with their own sets of constants p_0 and *a* for site and bond percolation, and were able to obtain a fairly good fit of p_c for a number of lattices of various dimensionality (with a fifth set of constants p_0 and *a* required for systems of very high dimensionality). Their class 1 contains all 2D lattices except the Kagomé lattice, while class 2 comprises all higher-dimensional systems plus the 2D Kagomé lattice.

Subsequently, van der Marck [8,22] considered a number of additional lattices, and argued that a formula of this type, depending only upon d and q, cannot be truly universal because of the existence of different lattices with quite different p_c but identical d and q. GM [20] responded that their formula is applicable only for "isotropic" lattices in which each site has the identical q. (Here we use "uniform" rather than "isotropic" to describe such lattices.) For nonuniform lattices, GM reformulated Eq. (5) by reinterpreting q to represent an effective coordination number q_{eff} (not necessarily the average value \bar{q}). Because q_{eff} cannot be found independently, this reinterpretation has the effect of turning their formula into a correlation between site and bond thresholds rather than predicting the actual values. This relation is developed further in Ref. [36] and discussed in Refs. [9, 37].

In Fig. 6 we plot our results using the same axes as GM, $\ln(1/p_c)$ vs $\ln(q-1)$ [21]. We also exhibit GM's predictions for their two classes of site percolation, which are straight lines on this plot. Many of the Archimedean lattices do not fall near either of GM's class, and the only way to obtain an accurate correlation for these lattices would be to introduce many more classes, clearly contradictory to the spirit of a universal formula.



FIG. 7. Percolation thresholds as a function of f, with the same symbols as in Fig. 6. The fit (solid line) is given in Eq. (10). Also shown is the correlation of Scher and Zallen [Eq. (6)] (dashed line).

D. A generalized Scher-Zallen correlation for p_c

Although an exact, truly universal formula for percolation thresholds in terms of a few lattice properties is undoubtedly out of the question, the development of approximate correlations is still useful for practical purposes. As shown in Fig. 6 and discussed in Refs. [8, 22], the coordination number q alone is not a good property for this purpose because of the large number of lattices of disparate p_c that share the same q.

We found that a much better correlation for the Archimedean lattices can be developed by relating p_c to the "openness" of the lattice structure as characterized by the density of sites ρ , which we define as the number of sites per unit area, taking the bond length as one for all bonds in the system and all polygons as regular (which is possible with all Archimedean lattices). For the Archimedean lattices, ρ turns out to be simply proportional to the well-known filling factor f introduced by Scher and Zallen [38], $f = \pi \rho/4$, where f is defined as the fraction of space occupied by disks of radius $\frac{1}{2}$ placed at each lattice site, again assuming unit bond length. To be consistent with previous work, we use the quantity f here also.

For four basic lattices in two dimensions, Scher and Zallen found good a good fit of p_c with the hyperbolic relation

$$fp_c \approx \text{const} = 0.44 \pm 0.02.$$
 (6)

However, applied to all 11 Archimedean lattices, this correlation proves to be quite poor, as shown in Fig. 7. On the other hand, this figure does show that a strong correlation (of a nearly linear form) exists between p_c and f. That is, fappears to be a good lattice property to use for a correlation for p_c , although not with the functional form of (6).

To find an expression for f for the Archimedean lattices, first consider the inverse of ρ , the area per site. The latter can be determined by drawing lines which bisect the centers of each polygon surrounding a given site, as in a dual-lattice construction, and summing the enclosed areas. The tiles defined by these bisector lines clearly fill the entire lattice, and the total area per site is simply one-third the area of each triangle, one-fourth the area of each square, etc., surrounding that site. Now, for Archimedean lattices with uniform bond lengths, all polygons are regular. The area of 1/nth of a regular *n*-gon, with unit edge length, is given by

$$A_n = \frac{1}{4} \cot \frac{\pi}{n}.$$
 (7)

For a lattice characterized by vertices $(n_1^{a_1}, n_2^{a_2}, ...)$, we then find

$$f = \frac{\pi}{4} \left[\sum_{i} a_{i} A_{n_{i}} \right]^{-1} = \pi \left[\sum_{i} a_{i} \cot \frac{\pi}{n_{i}} \right]^{-1}.$$
 (8)

The resulting values of f for the Archimedean lattices are listed in Table II.

The correlation between p_c and f shown in Fig. 7 is nearly linear and can be fit various ways. The linear leastsquares fit $p_c = 1.0405 - 0.5823f$ yields a rms error over the 11 Archimedean lattices of $\sigma_{11} = 0.0075$, while the quadratic fit

$$p_c = 0.9472 - 0.2777f - 0.2334f^2, \tag{9}$$

is somewhat better, with $\sigma_{11}=0.0054$. The small curvature in Fig. 7 can also be removed by plotting $p_c^2 \operatorname{vs} f$, yielding a slightly better correlation and containing only two parameters

$$p_c^2 = 0.9434 - 0.7637f, \tag{10}$$

TABLE II.	Values of p_c and la	attice characteristics f	for all 11	Archimedean	lattices. Δ	is the error wh	ien Eq. ((10) is use	1 to fit	the da	ita.
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Lattice	p_{c}	Ref.	q	f by Eq. (8)	$p_c^{\text{est.}}$ by Eq. (10)	Δ
$(3,12^2)$	0.807 904		3	0.3907	0.8031	0.0048
(4,6,12)	0.747 806		3	0.4860	0.7565	-0.0086
(4,8 ²)	0.729 724		3	0.5390	0.7292	0.0005
(6 ³) honeycomb	0.697 043		3	0.6046	0.6940	0.0030
(3,6,3,6) Kagomé	0.652 703 6	[15]	4	0.6802	0.6511	0.0016
(3,4,6,4)	0.621 819		4	0.7290	0.6218	0.0000
(4^4) square	0.592 746 0(5)	[16]	4	0.7854	0.5861	0.0066
(3 ⁴ ,6)	0.579 498		5	0.7773	0.5914	-0.012
(3 ² ,4,3,4)	0.550 806		5	0.8418	0.5482	0.0026
$(3^3, 4^2)$	0.550 213		5	0.8418	0.5482	0.0020
(3 ⁶) triangular	0.5	[15]	6	0.9069	0.5008	-0.0008



FIG. 8. Error from using GM's class 1 formula (\Box) , class 2 formula (Δ) , and our fit [Eqs. (8)–(10)] (\bullet), for the 18 lattices, plotted sequentially in the order they are listed in Tables II and III, respectively.

with $\sigma_{11}=0.0053$. Because of its relative simplicity and accuracy, we use this formula to fit $p_c(f)$, although Eq. (9) or even the linear fit could about as well have been used. The error cannot be reduced much further with a more complex fitting function, because of the inherent error in relating p_c to f, as discussed below.

The errors for each lattice resulting from Eq. (10), as listed in column Δ in Table II, are generally within about 0.01. This is in contrast to errors up to 0.05 if GM's correlations were used (taking the best class in each case). In Fig. 8 we plot the errors from using Eq. (10), and GM's universal formulas for the various lattices, clearly showing how GM's formulas are each accurate for certain lattices only, while Eq. (10) works fairly well for all of the lattices.

Interestingly, an excellent fit can also be made by using results from only the three lattices where p_c is known exactly (which happen to span the whole range of p_c values here): the triangular lattice ($p_c = 1/2$, $f = \pi\sqrt{3}/6$), the Kagomé lattice ($p_c = 1-2 \sin \pi/18$, $f = \pi\sqrt{3}/8$), and the (3,12²) lattice ($p_c = [1-2 \sin \pi/18]^{1/2}$, $f = \pi[7\sqrt{3}-12]$). A fit of these three points yields the quadratic equation

$$p_c = 0.946\,61 - 0.251\,03f - 0.266\,20f^2,\tag{11}$$

which produces an error of $\sigma_{11}=0.0062$, or, to the form of Eq. (10),

$$p_c^2 = 0.957\,28 - 0.780\,24f,$$
 (12)

with $\sigma_{11}=0.0058$. These formulas depend upon no Monte Carlo-measured values, and provide only slightly worse fits to the 11 Archimedean lattices than Eqs. (9) and (10), which were derived using all 11 lattices.

It turns out that the authors of Ref. [6] also proposed a correlation for p_c for the Archimedean lattices, closely related to ours. They compared p_c to a variable *m* which represents the average edge length of a minimally spanning tree on a complete lattice, normalized by the area. Because on the complete graph there is one edge per site, *m* is given by $m = \rho^{1/2} = (4f/\pi)^{1/2}$. Their plot of p_c vs *m* is more curved than the plot of p_c vs *f*, and they fit that curve by



FIG. 9. Five of the nonuniform lattices used to test the fitting formulas.

$$p_c = 0.685 + 0.799m - 0.899m^2$$
, (13)

which produces an error of $\sigma_{11}=0.0057$. Only a very slight improvement ($\sigma_{11}=0.005$ 69 vs 0.005 72) is obtained by adjusting their coefficients for our new, more precise, values of p_c . Clearly, various nearly equivalent ways of representing the relation of p_c to f can be found.

E. Extension to nonuniform lattices

So far we have considered the 11 uniform Archimedean lattices only. Many other regular and quasiregular lattices have been studied in the percolation field, and as a test of our correlation formula we apply it to some of those lattices as well.

When going to nonuniform lattices (referred to as anisotropic [21]), it is first necessary to come up with a prescription for calculating f. The density of sites idea becomes ambiguous for many lattices where it is not possible to assign unit length simultaneously to all the bonds of the system, and it is also not possible to keep the polygons regular. Because the threshold fundamentally depends upon the topological rather than geometric properties of the lattice, we define f by Eq. (8) with a_i taken as the *average* number of polygons of type n over the different nonequivalent vertices of the system. We call this the *generalized* filling factor.

Note that with nonuniform lattices, one could conceivably assign different values of p to the sites of different type. However, here we assume all sites are occupied with the same probability.

We looked at seven nonuniform lattices considered by van der Marck [8,9] and/or GM [21], and whose values of p_c are known (we did not determine any of these p_c here): the bowtie [42], bowtie dual, pentagonal, (4,8²)-covering, dice, Penrose, and Penrose dual lattices. The first five of these lattices are shown in Fig. 9, while the quasicrystalline Penrose and Penrose dual are shown, for example, in Refs. [39] and [21]. The form of the Penrose lattice used here is the rhomb or P3 form [25].

For the dice lattice, one-third of the vertices are (4^6) while two-thirds of them are (4^3) , so on the average the vertices are (4^4) . Likewise for the $(4,8^2)$ -covering lattice, we have $\frac{1}{3}(3^2,8^2) + \frac{2}{3}(3^2,4,8) = (3^2,4^{2/3},8^{4/3})$, for the bowtie

Lattice	<i>p</i> _c	Ref.	\overline{q}	f by Eq. (8)	$p_c^{\text{est.}}$ by Eq. (10)	Δ
$(4,8^2)$ -covering $(3^2,4^{2/3},8^{4/3})$	0.6768(2)	[8, 41]	4	0.6233	0.6836	-0.0068
bowtie dual $(4^{4/3}, 6^2)$	0.6649(2)	[8, 41]	$3\frac{1}{2}$	0.6548	0.6658	-0.0009
pentagonal (5 ^{10/3})	0.6476(2)	[9, 41]	$3\frac{1}{3}$	0.6848	0.6484	-0.0008
Penrose dual (see text)	0.6381(3)	[39]	4	0.7058	0.6359	0.0022
dice (4^4)	0.5848(2)	[8]	4	0.7854	0.5861	-0.0013
Penrose (4^4)	0.58391(1)	[39, 44]	4	0.7854	0.5861	-0.0024
bowtie (3 ³ ,4 ²)	0.5474(2)	[8, 41]	5	0.8418	0.5482	-0.0008

TABLE III. Data for nonuniform lattices. Here \bar{q} represents average vertex numbers.

lattice $\frac{1}{2}(3^4, 4^2) + \frac{1}{2}(3^2, 4^2) = (3^3, 4^2)$, for the bowtie dual lattice $\frac{1}{3}(4^2, 6^2) + \frac{2}{3}(4, 6^2) = (4^{4/3}, 6^2)$, and for the pentagonal lattice $\frac{1}{3}(5^4) + \frac{2}{3}(5^3) = (5^{10/3})$. For the Penrose lattice, the average vertices are simply (4⁴), while for the Penrose dual lattice the average vertices are [43] $(3^{a_3}, 4^{a_4}, 5^{a_5}, 6^{a_6}, 7^{a_7})$ with $a_3 = 3(x^2 + x^4) = 3(3 - 4x) = 1.583592135$, $a_4 = 4x^5 = 4(5x - 3) = 0.360679775$, $a_5 = 5(x^3 + x^6) = 5(4 - 6x) = 1.458980338$, $a_6 = 6x^7 = 6(13x - 8) = 0.206651122$, and $a_7 = 7x^6 = 7(5 - 8x) = 0.39009663$, where $x = (\sqrt{5} - 1)/2$ is the inverse of the golden ratio. Note that in general a_n satisfy $\sum_n(1 - 1/n)a_n = 1$ and $\sum_n a_n = \overline{q}$, where \overline{q} is the average coordination number.

These average vertex numbers are listed in Table III, along with p_c values, f values, $p_c^{\text{est.}}$, and error Δ from using Eqs. (8)–(10). Surprisingly, the Δ for these seven nonuniform lattices are generally smaller than the Δ for the Archimedean lattices, such that the rms error over all 18 lattices is reduced to σ_{18} =0.0045—even though our formula (10) for $p_c(f)$ was derived from the behavior of the 11 Archimedean lattices only. Even the Penrose dual lattice, which incorporates polygons with from three to seven sides and a very irregular structure, is also well described by Eq. (10). Evidently, the correlation between p_c and the generalized f is quite robust. The results for the nonuniform lattices are also included in Fig. 6, with \bar{q} substituted for q.

F. Discussion

One could conceivably use the additional data points from the nonuniform lattices to refine the fit of the formulas for $p_c(f)$ in Sec. III D. However, the improvement turns out to be marginal, implying that the (simpler) fit to just the Archimedean lattices is nearly optimal.

Note that if we had retained the definition of $\rho = 4f/\pi$ literally as the density of sites for these lattices, rather than using the definition (8) above, then the correlation between p_c and f for the nonuniform lattices would have been quite poor. An example is provided by the dice lattice, which in its usual representation has a site density identical to that of the triangular lattice, $2\sqrt{3}/3 = 1.1547$. The p_c for this lattice, 0.5851 [8], is substantially above the value for the triangular lattice, $\frac{1}{2}$, and the data point for this case would fall well above the line in Fig. 7.

A generalization of the Scher-Zallen filling factor for some nonuniform lattices was also considered in Ref. [40], whose approach was evidently to take a linear combination of the f's rather than of the a_n 's as we do here. For the dice and Penrose lattices, their method leads to the same f as ours, but for the Penrose dual lattice they find f=0.7106 in contrast to our value f=0.7058. Putting their f into Eq. (10) yields a somewhat poorer prediction $p_c=0.6330$ than ours, $p_c=0.6359$, compared with the measured $p_c=0.6379$.

While the generalized f is clearly a better lattice property than q for correlating p_c , it still cannot give exact results because there are lattices with identical f that have different p_c . However, in contrast to the situation with q, the p_c of lattices with identical f are in fact quite close together. For example, we have considered three different lattices with the average vertex environment of three triangles and two squares, corresponding to f = 0.8418: the two Archimedean lattices $(3^3, 4^2)$ and $(3^2, 4, 3, 4)$, and the nonuniform bowtie lattice. These lattices have site p_c 's of 0.550 806, 0.550 213, and 0.5475(8), respectively. For the two Archimedean lattices, the p_c 's are nearly identical, while the bowtie lattice, which has the same vertex numbers as the others on the average only, has a value of p_c that is lower by about 0.003. The deficiency in using q to correlate p_c also apparent, since the $(3^4, 6)$ lattice has the same q=5 as these three lattices, but a substantially higher $p_c = 0.579498$.

Another example occurs for the square $(p_c=0.592746)$, dice $(p_c=0.5848)$, and Penrose $(p_c=0.5839)$ lattices, whose (average) vertices are (4^4) in all cases (f=0.7854). Again, the p_c of these lattices are close to each other, with the nonuniform lattices having slightly lower values than the uniform one, with the "most" nonuniform one (the Penrose lattice) having the lowest p_c . And again, other lattices with q=4 but different average vertex numbers (there are four of them listed in Tables II and III) all have much different (in fact, much higher) values of p_c .

Note that van der Marck [23,41] pointed out that adding an extra site (with three bonds) at the center of any triangle on a 2D lattice does not change the value of p_c (site). If these extra sites are included in the calculation of f, then the predictions of Eq. (10) would now be rather poor. Therefore, one must disregard superfluous sites like these in our formulas. There are undoubtedly other types of lattices where our correlation will not work well.

As a final remark, we note that a further refinement of this type of fitting formula can be achieved by adjusting the values of A_n in Eq. (8) away from their regular polygon-based values—that is, treating A_n as a weight unrelated to the area formula. An attempt to do this led to a set of A_n in a somewhat smaller range than Eq. (7), an adjustment of Eq. (10), and an improvement of the overall fit to the 18 lattices from σ_{18} =0.0045 to 0.0028. However, because of the large num-

ber of adjustable parameters for a relatively small total number of lattices, this procedure is somewhat arbitrary, and the improvement over the polygon-based topological weights (8) is not so great. Thus, we conclude that the fit using the polygon-based area [Eq. (8)] is reasonable.

G. Conclusions

We have determined p_c (site) for the honeycomb and seven less-common Archimedean lattices to nearly six significant figures, about 100–1000 times more precise than previously known—except for the (3⁴,6) lattice, whose p_c was never determined previously, but bounded by a conjecture [34]. This work provides another demonstration of the efficiency of the hull-gradient method for determining p_c in two dimensions, as well as an additional check of the method's accuracy on a lattice with known p_c , the (3,12²) lattice.

We find a fairly good, nearly linear correlation between p_c and a generalization of the Scher-Zallen filling factor, although the accuracy of this correlation is far below what can be achieved in simulation. This correlation also works well on a number of nonuniform lattices, and is substantially more accurate than correlations based primarily upon coordination number, such as those of GM [17–19]. However, our result remains a correlation that is only approximate. Indeed, such a correlation based upon the vertex numbers alone can never be exact, since different lattices with identical vertex numbers ($a_1, a_2, ...$) are predicted to have identical p_c values, but their actual values differ (although by a relatively small amount).

All our results here are restricted to two dimensions and to site percolation. It would be interesting to see if a relation between p_c to the local topological environment can be extended to bond percolation as well as to higher dimensionality. (For bond percolation in two dimensions, the site covering lattice has no crossing bonds when q=3 and should work well with our correlations. However, for q>3, the covering lattice has crossing bonds, and (8) is not applicable.) It would also be interesting to explore the behavior of p_c (bond) on the Archimedean lattices.

Note added in proof. We would like to add a reference to the work of Ord and Whittington [45], who discuss bonddecoration transformations for percolation lattices. From this point of view, the result (4) for the threshold of the $(3,12^2)$ lattice can be derived by noting that the $(3,12^2)$ lattice is the covering lattice of a stretched-out honeycomb lattice, where each bond is replaced by two bonds in series. Then (4) follows immediately from p_c of the bond-honeycomb lattice. Secondly, in a recent work on site percolation on the square lattice [46], we find that the convergence of p_c^{est} to p_c is not linear but a higher power of $|\nabla p|$ (as indeed supported by



FIG. 10. Two orientations for the $(3^3, 4^2)$ and honeycomb lattices used to test the influence of lattice orientation in our method of determining p_c .

Fig. 4 here). However, this discovery doesnot affect our results here because we used very small gradients and did not have to extrapolate much at all. Finally, we note that d'Iribarne, Rasigni, and Rasigni have recently published an expanded report of their work on Archimedean lattices in Ref. [47].

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APPENDIX: IMPORTANCE OF GRADIENT ORIENTATION

In order to verify that the direction that the gradient is applied on a lattice has no effect on p_c , we calculated p_c for both the honeycomb and $(3^3, 4^2)$ lattices after they had been rotated 90°. Figure 10 shows the original orientation of the simulation and the orientation after the lattice has been rotated 90°. p_c for the honeycomb lattice was measured as 0.697 043(3) and then 0.697 046(3) after 90° rotation. Likewise, for the $(3^3, 4^2)$ lattice, p_c was measured as 0.550 213(3) and then 0.550 211(3) after 90° rotation. In both cases, the p_c values were identical within the error of the method, verifying that the orientation of the lattice has no effect on determining p_c in our method.

- J. V. Field, Vistas Astron. 23, 109 (1979); Arch. Hist. Exact Sci. 50, 241 (1997).
- [2] L. Fejes Tóth, Acta Math. 11, 363 (1960).
- [3] F. C. Frank and J. S. Kasper, Acta Crystallogr. 11, 184 (1958);
 12, 483 (1959).
- [4] H. Takeda and J. D. H. Donnay, Acta Crystallogr. 19, 474 (1965).
- [5] R. Shrock and S. H. Tsai, Phys. Rev. E 56, 2733, 4111 (1997).
- [6] C. d'Iribarne, G. Rasigni, and M. Rasigni, Phys. Lett. A 209, 95 (1995).

- [7] C. Dussert, G. Rasigni, and M. Rasigni, Phys. Lett. A 139, 35 (1989).
- [8] S. C. van der Marck, Phys. Rev. E 55, 1514 (1997); 56, 3732(E) (1997).
- [9] S. C. van der Marck, Int. J. Mod. Phys. C 9, 529 (1998).
- [10] T. Vicsek and J. Kertész, Phys. Lett. 81A, 51 (1981).
- [11] Z. V. Djordjevic, H. E. Stanley, and A. Margolina, J. Phys. A 15, L405 (1982).
- [12] B. Sapoval, M. Rosso, and J. F. Gouyet, J. Phys. (France) Lett. 46, L149 (1985).
- [13] M. Rosso, J. F. Gouyet, and B. Sapoval, Phys. Rev. B 32, 6053 (1986).
- [14] R. M. Ziff, P. T. Cummings, and G. Stell, J. Phys. A 17, 3009 (1984).
- [15] J. W. Essam and M. F. Sykes, J. Math. Phys. 5, 1117 (1964).
- [16] R. M. Ziff, Phys. Rev. Lett. 69, 2670 (1992).
- [17] S. Galam and A. Mauger, J. Appl. Phys. 75, 5526 (1994).
- [18] S. Galam and A. Mauger, Physica A 205, 502 (1994).
- [19] S. Galam and A. Mauger, Phys. Rev. E 53, 2177 (1996).
- [20] S. Galam and A. Mauger, Phys. Rev. E 55, 1230 (1997).
- [21] S. Galam and A. Mauger, Phys. Rev. E 56, 322 (1997).
- [22] S. C. van der Marck, Phys. Rev. E 55, 1228 (1997).
- [23] S. C. van der Marck, Phys. Rev. E 55, 6593 (1997).
- [24] S. C. van der Marck, J. Phys. A 31, 3449 (1998).
- [25] B. Grünbaum and G. C. Shephard, *Tilings and Patterns* (Freeman, New York, 1987).
- [26] R. M. Ziff and B. Sapoval, J. Phys. A 18, L1169 (1986).

- [27] R. M. Ziff and G. Stell (unpublished).
- [28] R. M. Ziff and P. N. Suding, J. Phys. A 30, 5351 (1997).
- [29] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed. (Taylor and Francis, London, 1994).
- [30] A. Weinrib and S. Trugman, Phys. Rev. B 31, 2993 (1985).
- [31] R. M. Ziff, Comput. Phys. 12, 385 (1998).
- [32] S. W. Golomb, *Shift Register Sequences* (Holden-Day, San Francisco, 1967).
- [33] N. Zierler, Inform. Control 15, 67 (1969).
- [34] P. Préa, Math. Comput. Modeling 26, 317 (1997).
- [35] I. Jensen and A. J. Guttmann, J. Phys. A 31, 8137 (1998).
- [36] S. Galam and A. Mauger, Eur. Phys. J. B 1, 255 (1998).
- [37] F. Babalievski, Phys. Rev. E 59, 1278 (1999).
- [38] H. Scher and R. Zallen, J. Chem. Phys. 53, 3759 (1970).
- [39] F. Yonezawa, S. Sakamoto, and M. Hori, Phys. Rev. B 40, 636 (1989).
- [40] F. Yonezawa, S. Sakamoto, and M. Hori, Phys. Rev. B 40, 650 (1989).
- [41] S. C. van der Marck (private communication).
- [42] J. C. Wierman, J. Phys. A 17, 1525 (1984); 21, 1487 (1988).
- [43] J. P. Lu and J. L. Birman, J. Stat. Phys. 46, 1057 (1987).
- [44] R. M. Ziff and F. Babalievski, Physica A (to be published).
- [45] G. Ord and S. G. Whittington, J. Phys. A 13, L307 (1980); 15, L29 (1982).
- [46] R. M. Ziff, Int. J. Mod. Phys. C (to be published).
- [47] C. d'Iribarne, M. Rasigni, and G. Rasigni, J. Phys. A 32, 2611 (1999).