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Percolation and Scaling on a Quasilattice†

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We report results of a study of percolation on a two-dimensional Penrose quasilattice. After an extensive numerical analysis, we find that two-dimensional universality is obeyed. The scaling exponents σ and τ have the values expected, $\tau = 2.04$ and $\sigma = 0.39$, consistent with the universality class for percolation on a 2D periodic lattice. But the percolation threshold $p_c = 0.483$, differs from other 2D lattices with the same average coordination number $\bar{z} = 4$.

KEY WORDS: Bond percolation; quasilattice; universality; critical exponents; threshold; connectivity; Penrose tiling.

1. INTRODUCTION

The recent discovery[1] of icosahedral quasicrystals, which exhibit a diffraction pattern with icosahedral symmetry known to be incompatible with periodicity, has generated much theoretical study of nonperiodic lattices[2]. However, so far, theoretical work is directed toward explanation of observed diffraction and electron microscopy patterns. Since the quasilattice is nonuniform in the short range, but globally homogeneous, and therefore intermediate in structure between periodic and random, it is worthy of further study.

In this paper we report on an extensive numerical study designed to investigate percolation on a quasilattice. First we review some geometrical properties of the Penrose 2D quasilattice (PL) relevant to percolation. Then we test the scaling theory of percolation on the lattice. According to the theory,[3] which treats the percolation problem as a general second-

† We dedicate this paper to the memeory of Marc Kac. One of us (J.L.B.) had the good fortune to known him on many levels: as friend, fellow scientist, and co-worker for human rights. His insight, wisdom, and compassion will remain with us as a lasting legacy of his life.

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order phase transition, critical behavior and critical exponents are independent of lattice structure. To date this has only been tested on periodic lattices.

In Section 2 we discuss the geometrical structure of the Penrose lattice, and the connection coefficients of vertices are given. The bond percolation threshold of the PL is examined in Section 3, and the result is interpreted in terms of the difference in the global connectivity of lattices. Then in Section 4 we give a detailed analysis of cluster statistics. The results are in agreement with the two-exponent assumption of the scaling theory of percolation. Critical exponents are found to be the same as those found on a periodic lattice. This confirms the universality prediction. In the last section we summarize the results and comment on future studies.

2. LATTICE STRUCTURE

There are many ways to obtain quasiperiodic lattices. Two equivalent methods are widely used, namely algebraic transformation and geometrical projection.[4] In this paper we will restrict ourselves to the two-dimensional

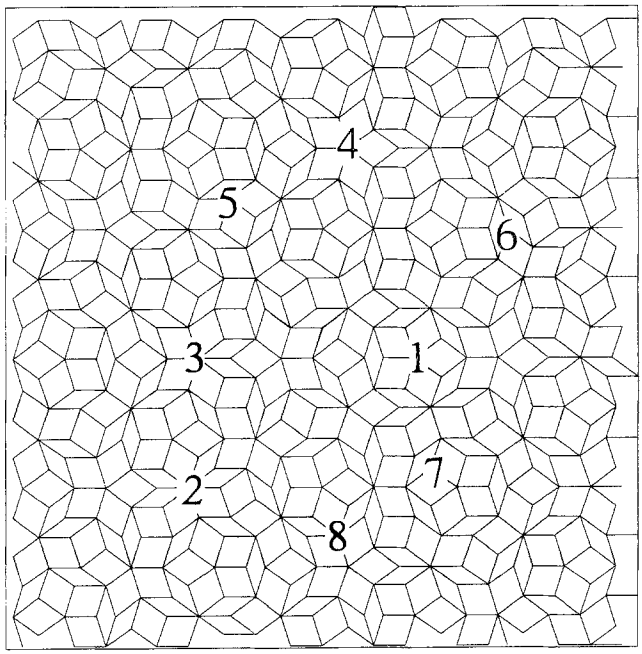


Fig. 1. A portion of a Penrose quasiperiodic lattice. There are eight different types of vertex, classified according to bond configuration. The ones labeled by 1–8 follow the labeling used in Eqs. (4) and (5). The average coordination number is 4 and there are twice as many bonds as vertices.

quasilattice with pentagonal symmetry known as the Penrose lattice (PL). Figure 1 shows a portion of the PL. It is a tiling of a plane by two different rhombuses in a nonperiodic fashion. There are eight different types of vertices in the PL if one classifies them in terms of their nearest neighbor configurations.[2] We label them as 1–8, respectively, as shown in Fig. 1 (these vertices previously have been given names such as sun, star, etc.). Each type of vertex has a different coordination number and appears in the PL with different frequency. The number of fat rhombuses is $\tau = (5^{1/2}+1)/2$ times larger than the number of thin ones. The orientation of these rhombuses is equally and uniformly distributed in the tenfold symmetry directions. This implies isotropic distribution of vertices and bonds.

Let $z(i)$ be the coordination number of the ith-type vertex, $\rho(i)$ be its frequency, and $\bar{z}$ the average coordination number. Let $p(i, j)$ be the frequency that a bond connects the ith type of vertex to the jth type of vertex. Then the following relations hold:

$$\sum_{i=1}^{8} \rho(i) = 1 \tag{1}$$

$$p(i, j) = p(j, i) \tag{2}$$

$$\sum_{i,j=1}^{8} p(i, j) = \sum_{i=1}^{8} z(i)\,\rho(i) = \bar{z} \tag{3}$$

From de Brujin's algebraic description[4] of the PL we derived the exact expressions[3]

$$\begin{aligned} &\rho(1) = \frac{1}{5^{1/2}\tau^5}, \quad \rho(2) = \frac{1}{\tau^6}, \quad \rho(3) = \frac{1}{\tau^7}, \quad \rho(4) = \frac{1}{5^{1/2}\tau^7} \\ &\rho(5) = \frac{1}{\tau^5}, \quad \rho(6) = \frac{1}{\tau^4}, \quad \rho(7) = \frac{1}{\tau^2}, \quad \rho(8) = \frac{1}{\tau^3} \end{aligned} \tag{4}$$

$$p(i, j) = \frac{1}{\tau^7} \begin{Bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 5^{1/2}\tau^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\tau & 4\tau & \tau \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5^{1/2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 2\tau^2 & 2\tau^2 \\ 0 & 2\tau & 1 & 0 & 0 & 0 & 0 & 2\tau^3 \\ 5^{1/2}\tau^2 & 4\tau & 2 & 0 & 2\tau^2 & 0 & 0 & 2\tau^4 \\ 0 & \tau & 3 & 5^{1/2} & 2\tau^2 & 2\tau^3 & 2\tau^4 & 0 \end{Bmatrix} \tag{5}$$

[2] Strictly speaking, there are only seven different types of vertex if one classifies according to the branching pattern of the vertex. However, for types 1 and 4 shown in Fig. 1, due to the totally different type of nearest neighbor vertex to which they are connected, they are treated as different.

[3] Equation (4) was derived independently in Refs. 5 and 6.

These results were confirmed numerically. A computer program has been developed to determine the interconnection of lattices. Simulation on the PL with sample size up to 50,000 lattice sites shows that the above equations are satisfied to order $(1/N)$, where N is the total number of lattice sites in the system. This shows that the distribution of vertices in the PL is uniform. In other words, the long-range fluctuation of the lattice structure is very small. On the other hand, the short-range fluctuation is very large, for example, the local coordination number and nearest neighbor configurations are quite different for different vertices, as is seen in Fig. 1.

Another important property of the PL is its local n-site configuration number $C(n)$, which is defined as the number of possible configurations in a block of n lattice sites (with fixed area).[7] The number $C(n)$ is constant for a periodic lattice and an exponential function of n for random lattice structures. It can be shown straightforwardly that for the Penrose lattice, $C(n)$ is linear in n. From this point of view the PL is a structure between the periodic and the random systems. But average quantities such as the coordination number, the appearance frequency of different types of vertices, and their orientation order are the same (to order $1/n$) for all those n-site configurations. So for those physical quantities that depend on long-range order only, the PL behaves much as a totally ordered system. This is crucial for understanding the results of percolation on PL.

3. PERCOLATION THRESHOLD

For the past two decades, percolation problems have been extensively studied both analytically and numerically. On the analytical side the scaling theory, which treats the percolation problem as a general second-order phase transition, has been quite successful, and numerical simulation on periodic lattices gives results in good agreement with theory. The Penrose lattice is the first example of a nonperiodic lattice with well-defined global symmetry and structure. Due to the nonperiodicity, the local structure of the lattice is nonuniform and fluctuates. So it provides an ideal lattice structure to test the scaling theory, because the critical behavior near the phase transition is a long-range fluctuation phenomenon. We have simulated the bond percolation on the PL extensively with a lattice system up to 50,000 lattice sites. In this section we first address the percolation threshold, and in the next section we discuss universality and critical exponents.

Recall that bond percolation means each bond in the lattice has probability p of being connected. The percolation threshold p_c is defined such that for $p > p_c$ there exists an infinite connected cluster, and below it

all clusters are finite. Qualitatively, one defines the percolation probability $P(p)$ as the probability that a randomly chosen bond is a connected bond belonging to the infinite cluster. Then

$$P(p)=0, \quad p<p_c; \qquad P(p)>0, \quad p\geqslant p_c \tag{6}$$

Figure 2 shows the result of simulation of $P(p)$ on the PL with 90,000 bonds. All data points are the result of an average of 20 runs, except for those close to p_c, which are the result of 50 runs average (see Fig. 4). We also have analyzed the finite-size scaling effect, with lattice size 500, 1000, 10,000, 40,000, and 90,000 bonds, which shows very good convergence of p_c with lattice size larger then 10,000 bonds. From details of all these studies and analysis of cluster distribution statistics around threshold (see next section), we conclude

$$p_c=0.483\pm 0.005 \qquad \text{bond percolation (PL)} \tag{7}$$

An infinite cluster is shown in Fig. 3.

As is well known, critical exponents are dimension-invariant, but the percolation threshold is different for different lattice structures. This is because it is the lattice structure, namely the connectivity, that determines p_c. An important quantity is the average coordination number of the lattice $\bar{z}$, which determines the local connection. For the 2D bond percolation,

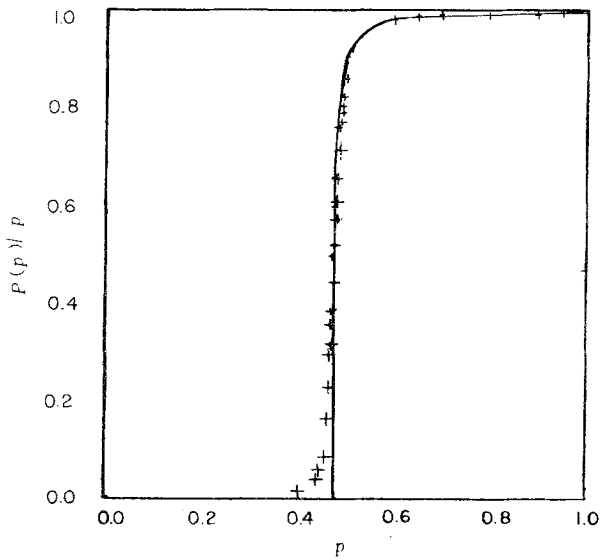


Fig. 2. Percolation probability $P(p)$ (normalized by the total number of connected bonds) as a function of p. (—) A guide to the eye; (+) simulation points. The lattice size is 90,000 bonds. All points are the result of taking 20 as a run average, except those very close to p_c, which are the result of a 50-run average.

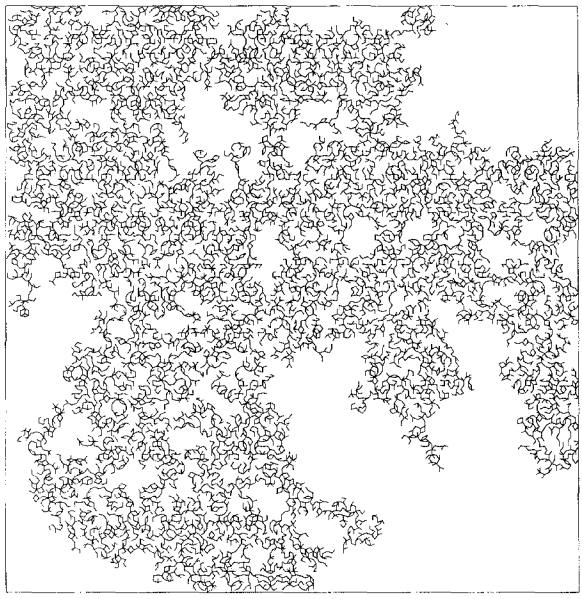


Fig. 3. An infinite cluster at $p=0.484$, which is just slightly above the threshold. The system size is 90,000 bonds.

it is known that $p_c\bar{z}\approx 2$ for triangular, square, and honeycomb lattices. However, for the Kagomè lattice,[8] which is periodic with coordination number 4 the same for all vertices, $p_c=0.45$. For the Penrose lattice, from Eqs. (3) and (4) one gets

$$\bar{z}=\sum_{i=1}^{i=8} z(i)\,\rho(i)=4 \tag{8}$$

but p_c for the Penrose lattice, as we found, is also smaller than that of the square lattice, but larger than that of the Kagomè lattice, though they all have the same average coordination number. Obviously $\bar{z}$ is insufficient to characterize the connection property of a lattice structure.

An important missing factor is that we did not take the global structure of the lattice into account. Since p_c is determined by the existence of an infinite cluster, which is a global structure, it is in general also dependent on the global connectivity of the lattice. Quantitatively, define $B(n)$ as the number of bonds to which a seed in the lattice can aggregate in n steps, with nearest neighbor hopping. For a lattice that is homogeneous over a large area (namely the average quantity has a meaning), one expects that for large n

$$B(n)=gn^d \tag{9}$$

in d dimensions. The proportionality constant g is a measure of global connectivity. In general it will be different for lattices with the same $\bar{z}$ but different lattice structure. For the case we are considering, namely $\bar{z}=4$ in $2D$, there are three lattices: Square (S), Kagomè (K), and Penrose (P). It is not difficult to obtain g for these lattices:

$$g(\mathrm{S})=\frac{\bar{z}^2}{4}=4; \quad g(\mathrm{P})=5-\frac{5}{2\tau^{-3}}=4.41; \quad g(\mathrm{K})=\frac{9}{2}=4.50 \tag{10}$$

where $\tau=(5^{1/2}+1)/2$ is the golden mean. Now compare with the percolation threshold:

$$p_c(\mathrm{S})=0.500; \quad p_c(\mathrm{P})=0.483\pm 0.005; \quad p_c(\mathrm{K})=0.449\pm 0.032 \tag{11}$$

we conclude that p_c is in general a decreasing function of g with fixed $\bar{z}$. For the quantitative relation between these quantities, more work needs to be done. This work is in progress.

4. CRITICAL EXPONENTS AND UNIVERSALITY[4]

The transition at percolation threshold is a second-order continuous phase transition. According to the modern theory of phase transitions the critical behavior near p_c is universal, in other words, it is independent of the details of lattice structure. Only the Euclidean dimension is a relevant quantity, which distinguishes different universality classes. Quantitatively, the scaling theory predicts that all critical exponents are the same for all lattices in the same dimension. Exponents are related by universality relations, and only two of them could be independent. Therefore, to test universality only two exponents need to be calculated.

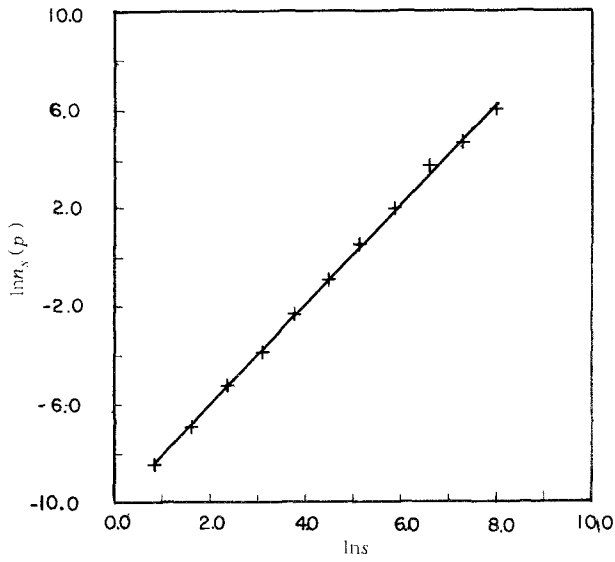
We have chosen to calculate cluster distribution exponents. The cluster-size distribution function $n_s(p)$ is defined as the average number of clusters each containing s occupied sites. Near the percolation threshold, the two-exponent assumption[3]

$$n_s(p) \propto s^{-\tau} f(z), \qquad z\equiv (p-p_c)\, s^{\sigma}; \qquad s\to\infty, \quad p\to p_c \tag{12}$$

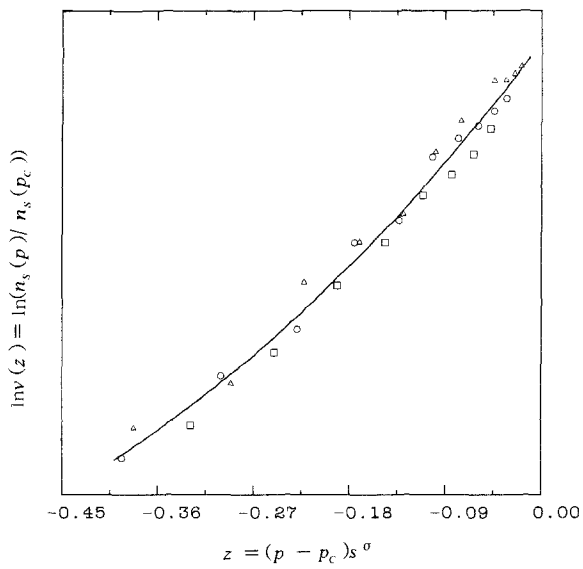
has been very successful and tested in periodic lattices. The usual critical exponents of percolation theory are related to τ and σ by

$$\alpha=2-\frac{\tau-1}{\sigma}, \qquad \beta=\frac{\tau-2}{\sigma}, \qquad \gamma=\frac{3-\tau}{\sigma}, \qquad \delta=\frac{1}{\tau-2} \tag{13}$$

[4] In this section we follow the usual convention in percolation theory and write τ for a critical exponent. This should not be confused with the "Golden Mean" used in Sections 1–3.



(a)



(b)

Fig. 4. (a) Log–log plot of cluster distribution function $n_s(p)$ as a function of cluster size (smashed, see text) at $p = 0.483$. A least squares fit gives the slope of the line as $\sigma = 2.04 \pm 0.04$. (b) Test of scaling, Eq. (12), very close to p_c. The exponents are taken from Eq. (13). Here $\ln v_s$ is plotted as a function of reduced variable z. Scaling requires that different symbols lie on a single curve. (△) $p = 0.47$, (○) 0.46, and (□) 0.45. All points are results of a 50-run average on the lattice with 90,000 bonds.

The best values of τ and σ obtained by bond percolation on a triangular lattice of 1.6×10^7 sites are[3]

$$\tau = 2.05, \qquad \sigma = 0.39 \tag{14}$$

Percolation around p_c on a Penrose lattice with 45,000 lattice sites was extensively simulated in our work. The primary restriction on the system size is the huge dynamic memory required for indexing the lattice. We calculated the cluster distribution function $n_s(p)$. In order to reduce fluctuations in statistics, we divide $n_s(p)$ into groups[3] with size interval from $s = 2^i$ to $2^{i+1} - 1$, $i = 0, 1, 2, \ldots$. For each group we took as the average s the geometrical mean of the upper and lower ends of the size interval. This approximation should be the better the closer n_s is approximated by an s^{-2} decay law. Figure 4 shows the results of cluster statistics based on 50 runs on a lattice with 45,000 vertices (90,000 bonds). We also did several simulations on different lattices (different members of the same local isomorphism class) of the same size, the results do not differ from one another. This is due to the small long-range fluctuation we discussed in Section 2., and the point is essential because for the infinite system all members of the same local isomorphism class are degenerate.

In Fig. 4a we plot $\ln n_s(p)$ against $\ln s$ at the percolation threshold $p_c = 0.483$. The slope of the straight line fit gives the exponent $\tau = 2.04 \pm 0.08$. Within the error bar it agrees very well with the known exponent [Eq. (14)]. In Fig. 4b we plot $\ln v(z) = \ln[n_s(p)/n_s(p_c)]$ against $z = (p - p_c)s^{\sigma}$ for different values of p. With $\sigma = 0.39$ one sees that all points fall on a single curve within a reasonable range. Therefore we conclude that percolation on a quasilattice belongs to the same universality class as percolation on a periodic lattice, and the critical behavior can be understood in the frame of scaling theory.

A side benefit of Fig. 4b is that this plot is an effective way to determine p_c. As one can see from Eq. (12), $\ln v(z)$ is 0 at $z = 0$. Furthermore, the deviation of $n_s(p)$ from $s^{-\tau}$ is different on the two sides of $z = 0$. For $z > 0$ ($p > p_c$), $n_s(p)$ decays more slowly than $s^{-\tau}$, which makes $\ln v(z)$ an increasing function of z. For $z < 0$ ($p < p_c$), $n_s(p)$ decays more rapidly than $s^{-\tau}$, and $\ln v(z)$ is a decreasing function of z. Therefore, by examining the deviation of $n_s(p)$ from the explicit exponential decay law, one can effectively determine the percolation threshold p_c.

5. CONCLUSIONS

In summary, we have analyzed the geometrical structure of the Penrose quasilattice. The connectivity structure of the lattice was analyzed and the connection coefficients given. Bond percolation on the Penrose

lattice has been studied. We found the percolation threshold $p_c = 0.483 \pm 0.005$. This is smaller than that of the square lattice and larger than that of the Kagomè lattice, though all of them have same average coordination number. We interpreted this in terms of a difference in the global connectivity in these lattices. Cluster statistics around p_c have been studied, and the results agree well with scaling theory. This is the first time that scaling theory has been explicitly tested on a nonperiodic lattice. Finally, we would like to point out that the short-range nonhomogeneity in the lattice structure of the Penrose lattice and its high orientational symmetry make it more closely resemble a real random medium.

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