

Reformulation of the percolation problem on a quasilattice: Estimates of the percolation threshold, chemical dimension, and amplitude ratio

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Percolation on a two-dimensional Penrose lattice is formulated using the distance between sites as the criteria for direct connections between occupied sites. The percolation threshold, chemical dimension, and amplitude ratio of the mean cluster size are estimated for this problem.

I. INTRODUCTION

The class of materials referred to as quasicrystals, which exhibit fivefold rotational symmetry and long-range order but do not have the full translational invariance of crystal systems,¹ play an important intermediate role between fully ordered crystal systems and disordered amorphous systems. The existence of magnetic ordering in some quasicrystal materials² is therefore of interest not only because of the technological importance of such materials, but also because it may offer insights into the nature of order-disorder transitions in amorphous materials. Magnetic ordering can exist only if the density of magnetic ions is greater than some percolation threshold which is dependent on the structure of the lattice. Indeed the percolation problem can be thought of as the low-temperature limit of a magnetic system.³ In this paper a study of percolation on a two-dimensional quasicrystal, the Penrose lattice (tiling), is reported.

Percolation on a Penrose lattice has previously been studied for bond percolation by Lu and Birman⁴ and by Yonezawa, Sakamoto, and Hori.⁵ In the formulation of the percolation problem used in this previous work a bond (direct connection) between two occupied sites exists if the bond corresponds to an edge of one of the rhombuses from which the lattice is constructed. In the present work the percolation problem is reformulated so that a bond between two sites exists only if the two sites are within a specified distance of each other. We may define a capture region consisting of a circle of specified radius around each site in the atom. A given site is connected by a bond to and only to those other sites within its capture region.³ This change in the formulation was motivated by the assumption that the direct interactions between magnetic ions in a real quasicrystal depend on distance rather than their relation to the mathematical construction of the lattice. The capture region formulation also has the advantage that it may easily be extended to any medium including a regular lattice or the continuum.

In Sec. II we describe the construction of the quasicrystal and the estimation of the percolation threshold p_c . In this work, the quasicrystal is a two-dimensional Penrose lattice. An implementation of the mean-field renormalization-group method using Monte Carlo

methods for large cells is used to obtain p_c . We also report the results obtained by this method for the test case of site percolation on the square lattice. The percolation threshold for the Penrose lattice is also obtained by an alternative Monte Carlo strategy.

In percolation theory, the fractal dimensions of the percolating cluster are of considerable interest. Section III reports results for the fractal dimension referred to as the chemical dimension. A study of a related quantity, the lacunarity, which describes the fluctuations in the mass density of the cluster as a function of chemical distance, is also described in Sec. III. Section IV describes results for the critical exponents β and γ and critical ratio of the mean cluster size amplitudes. A brief summary and comparison with other results are given in Sec. V.

II. PERCOLATION ON A QUASILATTICE

Several methods are available for constructing the two-dimensional Penrose lattice.⁶ For this work, the method was based on the construction of a pentagrid⁶ of 65 000 grid points. The required Penrose lattice is the dual of the pentagrid.⁶ Although the resulting lattice may be constructed by tiling the two-dimensional plane with two types of rhombus as originally described by Penrose,⁷ the tiling construction is not used here to define connections between lattice sites. Rather we assume that, in the simplest physical models, interactions, such as magnetic interactions, depend on the distance between sites in the lattice. Therefore bonds (direct connections) between sites in the Penrose lattice are defined as follows. For each site i define a capture region $\Gamma(i)$. A bond exists from site i to site j if and only if j lies within $\Gamma(i)$. In this work, the capture region $\Gamma(i)$ is taken to be a circle or radius $r = 1$. Here we use units in which the edges of the rhombuses in the Penrose construction have length 1. The seven types of vertex in the Penrose lattice which result from this construction are shown in Fig. 1.

The mean-field renormalization group⁸ has previously been applied to percolation for small cells on the square lattice.⁹ To lowest order in the effective mean field associated with sites adjacent to the cell, the mean-field renormalization-group equation can be written

$$f(p) = f'(p'), \quad (1)$$

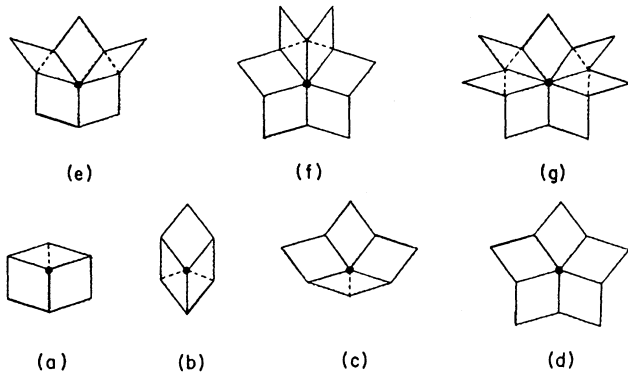


FIG. 1. Seven types of vertex in the Penrose lattice. Solid lines show the edges of the rhombuses. Dashed lines show additional bonds between sites within unit distance of each other.

where $f(p)$ is the sum over all sites adjacent to the cell of the probability that the adjacent site is connected to the origin (primed quantities refer to the larger cell in a given pair of cells). The resulting fixed point $p = p' = p^*$ is an estimate of the critical point of the system. Throughout this work, pairs of cells with linear sizes L and L' were chosen such that $L/L' \rightarrow 1$ as $L \rightarrow \infty$. As the cell size is increased the value of p^* is expected to approach the percolation threshold of the infinite system in the usual way predicted by finite-size scaling theory,¹⁰

$$p_c - p^* \propto L^{-1/\nu}. \quad (2)$$

For small cells $f(p)$ may be calculated analytically. However, for larger cells this rapidly becomes impractical. Consequently estimates of $f(p)$ were obtained at various values of p by using a Monte Carlo simulation. At a given value of p the estimate of $f(p)$ is taken to be the total number of sites adjacent to the cell connected to the origin averaged over the randomly generated configurations of occupied and unoccupied sites. The estimate of the fixed point p^* is then obtained from the crossing point of the two lines $f(p)$ and $f'(p')$ using a linear interpolation between the values of p closest to the crossing point.

As a test of this procedure it was initially applied to the square lattice in which sites are occupied with probability p . The fixed point values for various cell sizes are shown in Table I. In accordance with standard finite-size scaling arguments, we expect the value of p^* to approach p_c , as the linear size of the cell increases, as follows:

$$p^* = p_c + cL^{-1/\nu}, \quad (3)$$

where c is a constant and ν is known to be exactly $\nu = 4/3$.¹¹ The estimates of p^* were plotted against $L^{-1/\nu}$ and fitted to this linear form by a least-squares routine (see Fig. 2). Since the linear form is valid only for p^* sufficiently close to p_c , the values of p^* should, in principle, be fitted to a function containing correction terms:

TABLE I. Estimates of p^* from various pairs of cells on the square lattice.

L'/L	p^*
1.105 26	0.559 64
1.086 96	0.563 51
1.074 07	0.566 40
1.064 52	0.568 64
1.051 28	0.572 44
1.040 82	0.575 41
1.033 90	0.578 43
1.024 69	0.578 43
1.020 20	0.582 67

$$L^{-1/\nu} = c(p_c - p^*)[1 + A(p_c - p^*) + B(p_c - p^*)^{\Delta_1}], \quad (4)$$

where A and B are constants and $\Delta_1 \approx 1.25$.¹² To determine if the value of p_c obtained by fitting to the linear form is significantly affected by these correction terms a range of fit test was performed.¹³ The variation in the estimate of p_c as the number of data points is varied is shown in Table II. Although there is a slight overall upward trend in the first four values of p_c in this table, the shift in the central estimate of p_c remains comparable with the statistical error quoted in the table. Therefore it is unlikely that the effects of the statistical errors and correction terms could be reliably disentangled. Therefore, based on the results in Table II, we estimate

$$p_c(\text{square}) = 0.5929 \pm 0.0004, \quad (5)$$

in good agreement with previous estimates of $p_c = 0.5931 \pm 0.0006$ (Ref. 14) and $p_c = 0.5930 \pm 0.0001$.⁵ This provides some confidence in the application of the method to the Penrose lattice. [An alternative mean-field renormalization-group method which requires data from three different sized cells for each p^* (Ref. 15) was also tested on the square lattice. Although the estimates of p^* for small cells appeared to approach p_c more rapidly than

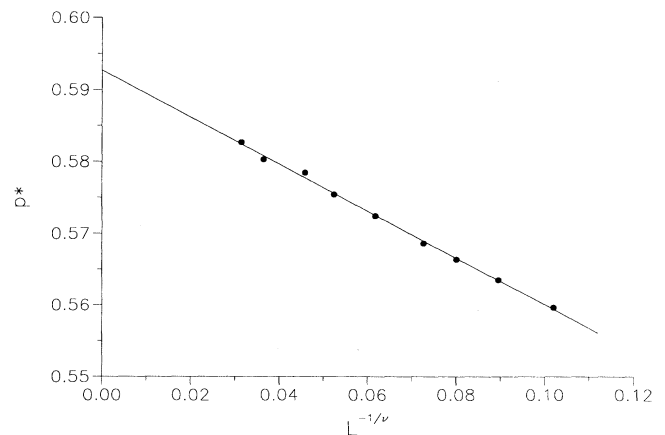


FIG. 2. p^* vs $L^{-1/\nu}$ for the square lattice.

TABLE II. Estimates of p_c for the square lattice, based on the N data points closest to p_c .

N	p_c
9	0.592 68±0.000 38
8	0.592 85±0.000 44
7	0.592 99±0.000 54
6	0.593 04±0.000 70
5	0.592 80±0.000 96

in the two-cell procedure, the estimates of p^* were very sensitive to the statistical errors in the Monte Carlo calculations and, consequently, the results could not reliably be extrapolated to the limit $L \rightarrow \infty$.]

In the square lattice all sites are equivalent. Consequently it is possible to choose any site in the square lattice as the origin and to average quantities over the randomly generated configurations of occupied and unoccupied sites. However, the Penrose lattice does not have local translational invariance and different sites cannot be treated as equivalent. Therefore, when working with finite cells, an average over possible choices of origin for the cell should be performed in order to avoid variations in the results due to a particular choice of the origin.¹⁶ In this work, the Monte Carlo simulation was performed on the Penrose lattice of approximately 650000 sites generated by the method described above. Estimates of $f(p)$ at chosen values of p were obtained, as described above for the square lattice, by averaging over the randomly generated configurations of occupied and unoccupied sites. However, for each such random configuration, an average of $f(p)$ was performed over possible choices of cell origin.¹⁶ For each cell size an average over about 2000 possible choices of origin was made for each random configuration. (The number of configurations was 100–200 at each value of p .) For the Penrose lattice circular cells of fixed radius were used. To allow for the averaging over different choices of origin, the value of L was taken to be

$$L = \sqrt{N_{\text{av}}} , \quad (6)$$

were N_{av} is the number of sites in the cell of given radius averaged over all choices of origin.

The analysis for the Penrose lattice follows that for the square lattice described above.¹⁶ Estimates of the fixed point for various pairs of cells are shown in Table III. The results are extrapolated to the large cell limit $L \rightarrow \infty$ by the finite-size analysis described above (Fig. 3). A range-of-fit test was again used to assess the effects of correction terms. The results are shown in Table IV. In this case there is no clear trend in the estimates of p_c and it may be assumed that the effects due to the correction terms are small compared with the statistical errors. From these results, we estimate

$$p_c(\text{Penrose}) = 0.5610 \pm 0.0006 . \quad (7)$$

As a check on our estimate of the percolation threshold for the Penrose lattice, an alternative Monte Carlo

TABLE III. Estimates of p^* for various pairs of cells on the Penrose lattice.

L/L'	L	p^*
1.0841	23.51	0.5294
1.0692	30.27	0.5336
1.0601	33.31	0.5362
1.0530	36.45	0.5367
1.0496	41.22	0.5395
1.0366	45.26	0.5408
1.0324	51.58	0.5432
1.0293	56.99	0.5445
1.0237	65.64	0.5458
1.0216	75.95	0.5469
1.0172	83.39	0.5485

strategy, which has previously been found to give good estimates of the percolation threshold for a variety of lattices,⁵ was used to estimate p_c for the Penrose lattice using the formulation of percolation theory described here. Following Ref. 5, three quantities are defined for a finite lattice of N sites: $R_N^D(p)$ is the probability there exists a cluster which spans the lattice from top to bottom, $R_N^R(p)$ is the probability that there exists a cluster which spans the lattice from left to right, and

$$R_N(p) = [R_N^R(p) + R_N^D(p)] / 2 . \quad (8)$$

The effective threshold $p_c(N)$ is then defined to be the value of p such that

$$R_N(p_c(N)) = 1/2 . \quad (9)$$

For five different values of p in the range [0.5600, 0.5620], 5000 Monte Carlo configurations were generated at each value of p and the corresponding value of $R_N(p)$ obtained. This was carried out for lattices of $N = 6000$, 12 300, and 31 600 sites. (In each case these lattices were “cut out” from a much larger lattice of $\approx 60\,000$ sites.)

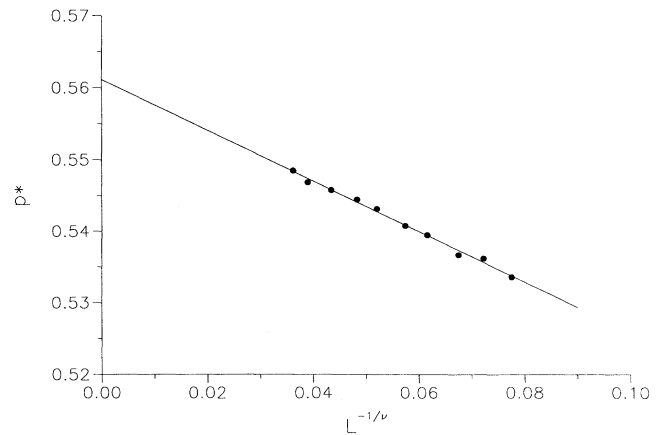


FIG. 3. p^* vs $L^{-1/\nu}$ for the Penrose lattice.

TABLE IV. Estimates of p_c based on the N data points closest to p_c .

N	p_c
11	0.5606 ± 0.0005
10	0.5611 ± 0.0006
9	0.5610 ± 0.0007
8	0.5615 ± 0.0007
7	0.5607 ± 0.0007
6	0.5605 ± 0.0009

The value of $p_c(N)$ in each case was then obtained by a linear interpolation between the points closest to $R_N(p)=0.5$ in each case. The results are shown in Table V. To extrapolate to $N \rightarrow \infty$ we again use a finite-size analysis. Assuming

$$p_c(N) = p_c + c\sqrt{N}^{-1/\nu}, \quad (10)$$

the values of $p_c(N)$ were fitted by a linear least-squares fitting routine. The resulting estimate of $p_c = 0.5611 \pm 0.0001$ is in excellent agreement with the value obtained by the Monte Carlo mean-field renormalization group. Therefore, although it is based on only three different finite lattices, this additional result provides some confidence in the estimate of p_c obtained for the Penrose lattice.

III. CHEMICAL DIMENSION AND LACUNARITY

The fractal dimensions which describe the geometry of the percolating cluster at the percolation threshold are of considerable interest in percolation theory and can be related to the physical properties of random systems. The fractal dimension known as the chemical dimension, D_f^c , is defined by

$$\langle M(l) \rangle \sim l^{D_f^c}. \quad (11)$$

In this definition, l , the chemical distance, is the number of steps on the cluster required to reach a given site from the origin. $M(l)$ is the total number of occupied sites at chemical distance less than or equal to l from the origin.

The Monte Carlo algorithm used here generated clusters, at the percolation threshold value $p = p_c = 0.561$, starting from a specified origin on the Penrose lattice constructed as described above. The algorithm is a modified Leath algorithm in which the neighbors of sites already in the cluster, but not yet tested to determine if they are occupied, are stored in an array. The sites in

TABLE V. Estimates of $p_c(N)$ for various lattice size N for the Penrose lattice using the Monte Carlo strategy of Ref. 5.

N	$p_c(N)$
6 000	0.560 72
12 300	0.560 85
13 600	0.560 89

this array are tested in the next cycle of the algorithm to determine if they are occupied and if they are they are added to the cluster. Consequently, the cycle of the algorithm at which a given site is added to the cluster is equal to the chemical distance of that site from the origin. $M(l)$ was calculated, using this method, for various choices of origin. The average $\langle M(l) \rangle$ in the definition of D_f^c was then taken to be an average over possible choices of origin, as well as an average over configurations of occupied and unoccupied sites, to allow for local variations in the connectivity due to the choice of origin. In this averaging process, clusters which reached $l=200$ were considered to be percolating clusters while clusters which terminated before they reached this value of l were discarded from the average. A log-log plot of $\langle M(l) \rangle$ vs l is shown in Fig. 4. From the slope of the least-squares fit to the points on this plot we obtain $D_f^c = 1.621 \pm 0.001$.

The maximum chemical distance considered in this analysis was $l_{\max} = 200$. To access the possible finite-size effects, the analysis was repeated with maximum chemical distances of $l_{\max} = 100, 125, 150,$ and 175 . The results are shown in Table VI. There is a clear upward trend as l_{\max} increases. In Fig. 5, $D_f^c(l_{\max})$ is plotted against l_{\max}^{-1} . A straight-line extrapolation of this data to $l_{\max} \rightarrow \infty$ provides our estimate of

$$D_f^c = 1.646 \pm 0.005. \quad (12)$$

The chemical dimension discussed above describes how the average number of sites, in the percolating cluster, connected to the origin varies as the chemical distance increases. However, since the clusters are random objects, there will be fluctuations about this average. The magnitude of these fluctuations is measured by the lacunarity¹⁷ \mathcal{L} defined by

$$\mathcal{L} = \Delta M(l) / \langle M(l) \rangle, \quad (13)$$

where

$$\Delta M(l) = (\langle M(l)^2 \rangle - \langle M(l) \rangle^2)^{1/2}. \quad (14)$$

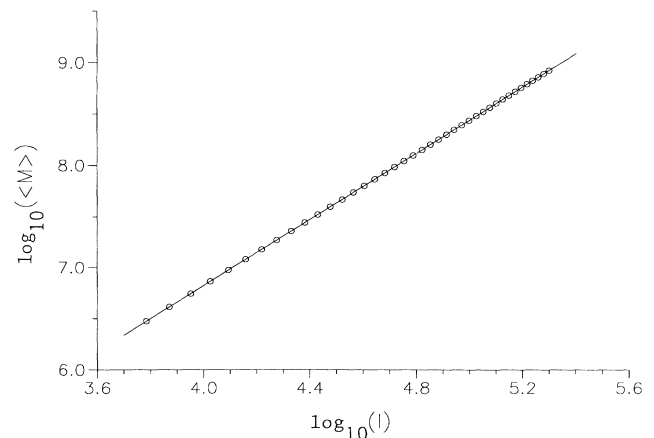


FIG. 4. Log-log plot of $\langle M(l) \rangle$ vs l .

TABLE VI. Estimates of D_f^c for various values of l_{\max} .

l_{\max}	D_f^c
100	1.595 ± 0.003
125	1.606 ± 0.002
150	1.612 ± 0.002
175	1.617 ± 0.002
200	1.621 ± 0.001

Here the averages denoted by $\langle \rangle$ are again interpreted as averages over both the Monte Carlo configurations and the choice of origin in the case of the Penrose lattice.¹⁶ Plots of \mathcal{L} vs chemical distance l for various values of p are shown in Fig. 6. As for regular lattices,¹⁷ each curve is almost horizontal for small values of l , but decreases more rapidly after a turning point is reached. The value of l at which the turning point occurs depends on the value of p . For values of l beyond the turning point the lacunarity decreases and each of the curves follows approximately the same power law

$$\mathcal{L} \propto l^{-\vartheta}, \tag{15}$$

where

$$\vartheta = 1.01 \pm 0.02. \tag{16}$$

Moreover, at $p = p_c$ the lacunarity does not exhibit the turning point but remains almost constant over the range of l studied.

This is consistent with the assumption that the turning point occurs when the chemical distance is of the same magnitude as the pair-connectedness length.¹⁷ For $l \ll \xi$ there are large fluctuations in the number of sites connected to the origin, due to the structure of the percolating cluster. However, for $l \gg \xi$ the sites are homogeneously spread through the system and it is expected that $M(l) \sim l^d$ and $\Delta M(l) \sim l^{d/2}$. Consequently, for a two-dimensional system, $\mathcal{L} \sim l$ at large values of l .

The limiting value of the lacunarity when $p = p_c$ is approximately 0.38 in good agreement with the values found for regular lattices,¹⁷ confirming the universality of the lacunarity.

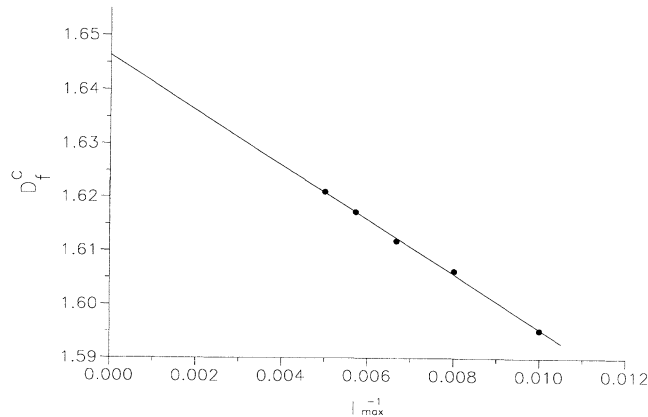


FIG. 5. Estimates of D_f^c vs l_{\max}^{-1} .

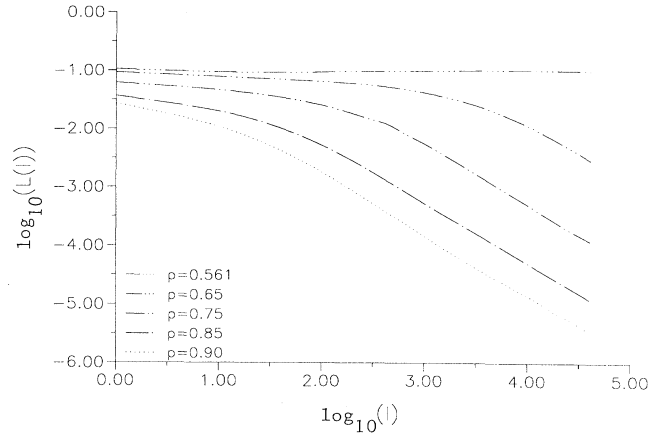


FIG. 6. Lacunarity vs chemical distance for various values of p .

IV. CRITICAL EXPONENTS AND THE AMPLITUDE RATIO

A detailed study of percolation on a triangular lattice has previously been performed by Hoshen *et al.*¹⁸ Here we apply a similar analysis to the Penrose lattice. A finite Penrose lattice, of approximately 56 000 sites, with a circular boundary was “cut” from the larger lattice generated from a pentagrid as described in Sec. II. Cluster statistics were then obtained from Monte Carlo simulations for p in the ranges $[0.490, 0.535]$ and $[0.595, 0.640]$.¹⁶ For each value of p considered, 4000–10 000 configurations of occupied and unoccupied sites were generated. The mean number of sites in the largest cluster

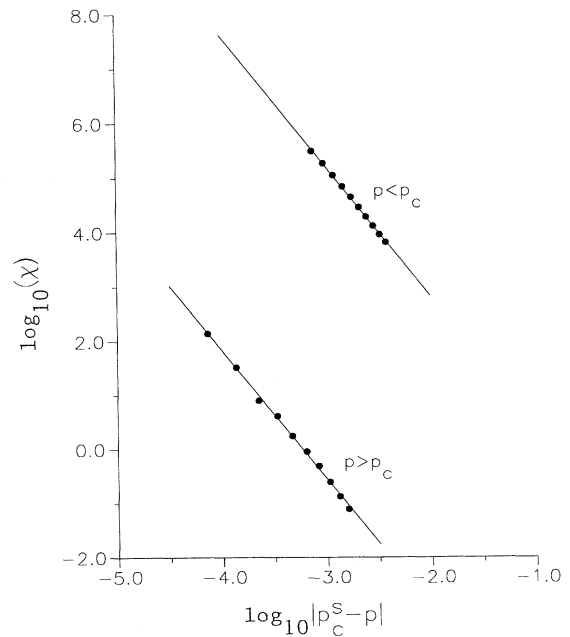


FIG. 7. Log-log plot of χ vs $|p_c^s - p|$ at $p_c^s = 0.579$.

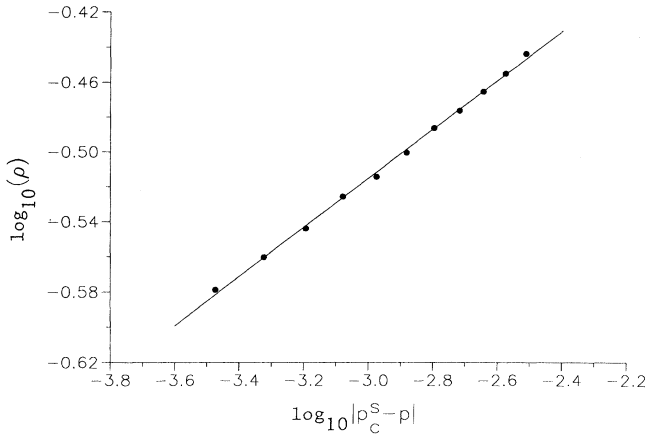


FIG. 8. Log-log plot of ρ vs $|p_c^s - p|$ at $p_c^s = 0.579$.

ter, ρ , and the second moment of the cluster number distribution

$$\chi = \sum_s s^2 n_s, \quad (17)$$

where n_s is the mean number of clusters of size s per site (the largest cluster is excluded from this sum), were calculated at each value of p .

The critical exponents β and γ and the amplitude ratio R are defined by

$$\rho = A |p_c - p|^\beta, \quad p \rightarrow p_c^+, \quad (18)$$

$$\chi = C_- |p_c - p|^{-\gamma}, \quad p \rightarrow p_c^-, \quad (19)$$

$$\chi = C_+ |p_c - p|^{-\gamma}, \quad p \rightarrow p_c^+, \quad (20)$$

$$R = C_- / C_+. \quad (21)$$

Following Ref. 18 we assume that the finite size of the lattice can be partially compensated for by replacing p_c in the above definitions by a shifted effective threshold p_c^s . The value of p_c^s to be used is found by adjusting the trial value until the values of γ obtained from the slopes of log-log plots of χ vs $|p_c^s - p|$ are the same for the data with $p > p_c$ and the data with $p < p_c$ (see Fig. 7). From this procedure the following values are obtained:

$$p_c^s = 0.579, \quad (22)$$

$$\gamma = 2.39 \pm 0.03, \quad (23)$$

$$R = 310 \pm 60. \quad (24)$$

Using this value of p_c^s , β is obtained from the slope of a log-log plot of ρ vs $|p_c^s - p|$ (see Fig. 8). This procedure results in the value

$$\beta = 0.140 \pm 0.002. \quad (25)$$

V. SUMMARY

Percolation on a Penrose lattice in which bonds are determined by the distance between lattice sites has been

studied. The percolation threshold $p_c = 0.5610 \pm 0.0006$ was determined by using a Monte Carlo implementation of the mean-field renormalization-group technique. As a test of this method, p_c was also estimated for the square lattice and excellent agreement with results from other methods was obtained. A further check was provided by using an alternative Monte Carlo strategy to determine p_c for the Penrose lattice. This, although only based on three finite lattice calculations, gave excellent agreement with the mean-field renormalization-group result.

The chemical dimension, critical exponents β and γ , and the critical amplitude ratio have been calculated using Monte Carlo techniques for the Penrose lattice. All of these quantities are universal in the renormalization-group sense and therefore should be the same for any medium (regular lattice, quasicrystal, or continuum).

The value of the chemical dimension $D_f^c = 1.646 \pm 0.005$ obtained in this work is consistent with previously obtained results for a regular lattice of 1.64 ± 0.02 .¹⁹ However, D_f^c may be related to the fractal dimension d_{\min} defined by

$$l \sim r^{d_{\min}}, \quad (26)$$

where r is the Pythagorean distance. From this definition,

$$D_f^c = D_f / d_{\min}, \quad (27)$$

where $D_f = 1.89$ is the fractal dimension of a two-dimensional percolation cluster.²⁰ A large-scale simulation gives a value of $d_{\min} = 1.30 \pm 0.002$ and hence $D_f^c = 1.678 \pm 0.003$.²¹ The difference between these results may be due to finite-size effects.

The values of $\beta = 0.140 \pm 0.002$ and $\gamma = 2.39 \pm 0.03$ obtained in this work are in excellent agreement with the known exact values $\beta = 5/36 \approx 0.139$ and $\gamma = 43/18 \approx 2.39$.²² The ratio of critical amplitudes for the mean cluster size has proved to be a difficult quantity to estimate accurately and has been the subject of some controversy.²³ The value obtained for the Penrose lattice in this work, $R = 310 \pm 60$, is somewhat higher than that obtained in an extensive study of a triangular lattice of 4000×4000 sites which found $R = 196 \pm 40$ using a similar analysis.¹⁸ R may also be estimated from data in the book by Stauffer.²⁴ The central estimate of R obtained from this data, by a similar analysis, is ≈ 300 but with substantial error bounds of ≈ 170 . The error bounds on R , in this work, represent only the statistical error in obtaining C_+ and C_- from linear fits to log-log plots of the data. In view of this, the discrepancy between the lower limit allowed by the error bars for the Penrose lattice and the upper value allowed by the error bars for the triangular lattice is probably not a significant contradiction of the assumed universality of R . However, in a study of percolation on an amorphous system it was found that $R \approx 14$.²⁵ It seems likely, in view of the results quoted above, that this significantly lower value is a result of finite-size effects and statistical errors and is not an intrinsic property of the randomness of the system studied. (The linear size of the system studied was ≤ 60 and the average appears to have been taken over samples of only 20–40 configurations. However, it should be noted that

this work was done at a density of 10 sites/unit area and, therefore, a system of linear size 60 contains 36 000 sites.)

This work was motivated by the need to formulate a percolation model suitable for describing critical phenomena in quasicrystals. With systems such as magnetic quasicrystals in mind, a formulation in which the existence of a bond between two sites is dependent on the distance between the sites was used. This capture region formulation can be equally well applied to percolation in the continuum or on a regular lattice. It therefore provides a natural way to view the quasicrystal as intermediate between the regular lattice and an amorphous system. The work reported here could be extended in several ways. The present mean-field renormalization-group analysis could be extended to determine how p_c depends on the radius of the capture region. The percolation model could be modified to allow different types of site in the quasicrystal to have different probabilities of being occupied by a magnetic ion. Experimental studies pro-

vide some evidence that this is the case in real quasicrystal systems.²⁶ Perhaps most importantly, because the formulation of the percolation problem does not depend on the mathematical construction of the quasicrystal and because the pentagrid method of constructing the quasicrystal can be extended to three dimensions the work reported here could, in principal, be extended to three-dimensional quasicrystal systems. However, this would require considerable computational resources since a list of the sites in the quasicrystal and their bonds must be stored during the Monte Carlo computations.

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