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COORDINATION NUMBER AND BOND PERCOLATION

by

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ABSTRACT

For some d-dimensional lattices, we show that $\frac{1}{z} + \frac{1}{z^D} = \frac{1}{d}$, where z and z^D are coordination number of a lattice and its dual, respectively. In two dimension, we show that the weighted average of zp_c for the triangular and hexagonal lattices satisfies a universality hypothesis. In dimensions $d \geq 3$, the universality hypothesis implies a duality transformation.

Key-words: Dual lattices; Bond percolation; Universality hypothesis.

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In the previous work, we have extended the concept of duality to three dimensions and shown that the fcc and diamond lattics are dual to each other (Chao 1982a). In this Letter, we show a possible way for constructing a particular type of dual lattices in hyperspace and establish a relation for the coordination number between such lattices. A duality transformation for bond percolation in d dimensions is shown to be the consequence of a universality hypothesis.

In three dimensions, a dual lattice is defined as the lattice formed by connecting the sites that are placed at the center of each elementary polyhedron on the original lattice. A dual lattice in d dimensions can be considered as that formed by connecting sites placed at the center of each d-dimensional elementary polyhedron on the original lattice (Wegner 1971). Although it is difficult to visualize lattices in hyperspace, we can still discuss a particular type of dual lattices that is analogous to the triangular and hexagonal, as well as the fcc and diamond lattices.

The simplest regular polyhedral in d dimensions is consisted of d+1 bonds incident from a common point. We assume that there exists d-dimensional lattice that can be covered by such polyhedrals; then the coordination number of this lattice is

$$z = d + 1. \qquad (1)$$

The structure of such a lattice can be visualized as

repetition of polyhedrals such that each of the end points of a constituent polyhedral is connected to those of the other d polyhedrals. From this lattice, we can obtain its dual by using a transformation similar to the star-triangular and tetrahedral-pyramid transformations (Chao 1982a), i.e., we decimate the sites at the center of each constituent polyhedral and connect the remaining sites by new bonds. Thus, each constituent polyhedral on the original lattice is replaced by a regular polyhedron with d+1 conners on the new lattice. This new lattice is the dual of the original one, since its constituent polyhedron is the dual of the corresponding polyhedral. Therefore, each bond on the original lattice is now replaced by d bonds on the dual lattice, because there are d bonds joining a conner of such d dimensional polyhedron to the other d conners. Thus, the coordination number of the dual lattice is

$$z^D = zd = d(d+1). \qquad (2)$$

From (1) and (2), we obtain a simple relation between coordination numbers for the dual lattices:

$$\frac{1}{z} + \frac{1}{z^D} = \frac{1}{d} \qquad (3)$$

This relation can readily be verified for the triangular-honeycomb and fcc-diamond lattice pairs. Furthermore, it is consistent with z=2d for the square, simple cubic and hypercubic lattices that are self-dual. Therefore, eq. (3) is more general than just for the particular dual pair we are considering. Because of the importance of coordination number in determining the percolation threshold for bond percolation on a lattice, we expect that (3) to be useful for studying bond percolation.

For bond percolation, it has been observed by Vyssotsky et al (1961) that the product of z with the percolation threshold p_c is approximately constant for lattices in d=2 and 3 through the following relation:

$$zp_c \simeq \frac{d}{d-1} . \qquad (4)$$

Therefore, the mean number of bonds per site, zp_c, required for the onset of percolation seems to be universal to some extend. Table 1 shows that zp_c is exactly 2 for the square lattice and differs from this value by about 0.04 and 0.08, respectively, for the honeycomb and triangular lattices. It is therefore puzzling why the approximation (4) becomes exact for the square lattice but gives large errors for the other two-dimensional lattices. Based on (3), we show in the following that a universal relation for zp_c can be established with respect to dual lattices.

Consider the duality transformation which can be written as

$$p_c + p_c^D = 1, \quad \text{for} \quad d = 2. \tag{5}$$

Now, we divide (5) by (3) to yield

$$\frac{z^D(zp_c) + z(z^D p_c^D)}{z+z^D} = 2, \text{ for } d=2. \tag{6}$$

Thus, the weighted average value of $^{z}p_c$ for the two-dimensional dual lattices satisfies universality. The validity of (6) is readily verifiel for the triangular-honeycomb lattice pair as well as for the self-dual square lattice.

In d dimensions, the universality hypothesis can be written as

$$\frac{z^D(zp_c) + z(z^D p_c^D)}{z+z^D} \simeq \frac{d}{d-1} . \tag{7}$$

Unfortunately, we cannot make an exact verification of (7) for $d \geq 3$, since exact values for p_c are not available. Nevertheless, if we use the estimated values list in Table 1 for the diamond and fcc lattices, we obtain 1.5201 for the left-hand side of (7). Thus, the discrepancy from universal value (1.5 for d=3) for the weighted average is considerably smaller than that for each individual value for the fcc and diamond lattices illustrated in Table 1. For simple cubic lattic, $zp_c = 1.4952$ using $p_c =$

0.2492 ± 0.0002 (Wilke 1983).

The universality hypothesis (7) implies a duality transformation

$$p + p^D = \frac{1}{d-1} , \quad (p, p_D \leq \frac{1}{d-1}) \tag{8}$$

which leads to

$$p_c = \frac{1}{2(d-1)} , \tag{9}$$

for simple hypercubic lattices. Equation (9) has also been discussed recently by Kirkpatrick (1979) and by Chao (1982b). In fact, the p_c values predicted by (9) are only slightly higher than those estimated from series expansion of Gaunt and Ruskin (1978) by 0.003 to 0.007 for d = 3 to 7. Gaunt and Brak (1984) have pointed out that the expansion of (9) with the parameter $\sigma = 2d-1$ does not agree with that of Gaunt and Ruskin (1978). It is therefore interesting to try to understand to what extend our hypothesis may be valid for $d \geq 3$.

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TABLE 1

lattice	z	p_c	zp_c
square	4	0.5	2
triangular	6	0.3473	2.0828
honeycomb	3	0.6527	1.9581
sc	6	0.2492	1.4952
fcc	12	0.1185	1.4220
diamond	4	0.3882	1.5528

Table 1. The coordination number z, bond percolation threshold p_c and mean number of bonds per site for the onset of percolation zp_c for some two-and three-dimensional lattices. The value of p_c for sc is the Monte Carlo estimate of Wilke (1983); fcc is the estimate of Cox and Essam (1976) and diamond lattice is taken from Essam (1972).

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