Polychromatic percolation: Coexistence of percolating species in highly connected lattices

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A generalization of percolation from a two-species (black-and-white) random process to a multispecies (polychromatic) process has been developed. The division of the chromatic composition field into regions in which different numbers of colors percolate for C colors on a lattice with percolation threshold p_c has been analyzed. A panchromatic regime (all species percolate) occurs when $C < p_c^{-1}$, occupying a fraction $(1-Cp_c)^{C-1}$ of the composition field. Since polychromatic percolation has greatest scope for highly connected low-p_c lattices, these ideas have been applied to site-percolation processes on d-dimensional close-packed lattices, as well as $d = 2$ and $d = 3$ lattices with long-range interactions. Also the concept of a lattice-independent dimensional-invariant critical volume fraction for site percolation has been extended to $d = 4$ and $d = 5$, but is shown to fail for $d > 8$. Possible applications of polychromatic percolation are briefly discussed.

I. INTRODUCTION

Percolation theory[1,2] continues to develop rapidly and fruitfully, primarily because it provides a well-defined, but nevertheless transparent and intuitively satisfying, geometrical model for spatially random phenomena. It has been applied to a diverse (and growing) collection of physical situations which includes, *inter alia*, dilute ferromagnets,[3] polymeric gels,[4] amorphous semiconductors,[5] random-resistor networks,[6] and microscopically inhomogeneous materials.[7] Among the most recent developments has been the mapping onto percolation theory of the renormalization-group approach which has been so successfully applied to the theory of phase transitions,[8] as well as the comparison of the critical dimensionalities (above which mean-field theory applies to the critical exponents) in the two theories.[9-11]

The standard formulation of percolation theory is obtained by associating a nongeometric property (or state) with each of the sites (vertices) or bonds (connections between sites, usually, but not necessarily, limited to pairs of sites which are nearest neighbors) of a regular periodic geometric lattice. The nongeometric property, which is randomly assigned to each site or bond and which carries the statistical character of the problem, *is usually assumed to take on only two values.* Thus, in site-percolation processes, each site is either *filled* or *empty* (with probabilities p and $1-p$, respectively), while in bond percolation, each bond is either *unblocked* or *blocked* (with corresponding probabilities). Adjacent filled sites (or unblocked bonds) are regarded as linked, and when p exceeds a critical value p_c (the critical probability, critical concentration, or percolation threshold) the clusters of linked sites (or bonds) are no longer all isolated and an infinitely extended cluster appears. It is the occurrence of this critical behavior at p_c which has made the percolation process an attractive model for the physical situations cited above.

In this paper, we develop a generalization of percolation theory in which the randomly assigned nongeometric property may take on three or more discrete values, rather than just two. We shall refer to this situation as *polychromatic percolation.* This is in close analogy to the generalization which occurs in group theory on passing from the Shubnikov black-and-white symmetry groups to the Belov groups of colored symmetry.[12] Another analogy is the transition from spin $\frac{1}{2}$ and multiplicity 2 to higher spin and multiplicity ≥ 3.

The possibility of having many colors or species present, rather than just two, is most interesting in situations in which the percolation threshold is low, since in such cases it is possible for several species to simultaneously possess concentrations which exceed p_c. Only lattices which are highly connected (i.e., which provide an abundant supply of interconnecting bonds per site) can exhibit low values of p_c and thereby permit the coexistence of several interpenetrating, unbounded clusters of different colors. In this paper, it will suffice to use the simplest measure of connectivity, the coordination number z specifying the number of neighboring sites to which each site is connected.

There are two basic ways in which to obtain lattices with arbitrarily high connectivity. For simple lattices with connections restricted to nearest neighbors only, a technique for indefinitely increasing the number of bonds per site is to consider the given type of lattice in higher-dimensional spaces. For lattices in two and three dimensions, progressively increasing the interaction range by introducing bonds to more distant neighbors has the same effect. Both types of highly connected lattices will be discussed here as vehicles for polychromatic percolation. For concreteness and simplicity, the specific cases considered will deal mainly with site percolation, but the trends and ideas involved carry over to bond percolation also.

Polychromatic percolation in general is analyzed in Sec. II, with emphasis on the composition field and its partition into regions in which different species percolate (or all do, or none; two situations of special interest). Percolation properties of close-packed lattices in higher dimensions are discussed in Sec. III, in preparation for the application of the results of Sec. II. While p_c is now known for site-percolation processes on d-dimensional simple cubic lattices, it is not known for the close-packed lattices. Estimates for the latter are developed, for the first time, in Sec. III B. As a prerequisite for these estimates, in Sec. III A we deal with the validity of extending to higher dimensions the concept of a critical volume fraction in site-percolation processes. We find that this construct retains its validity for $d=4$ and $d=5$, but fails to be valid for $d>8$. A quantitative description of the scope for multiple percolation on higher-dimensional lattices is given in Sec. IV A, and a corresponding discussion for site-percolation processes on highly connected two- and three-dimensional lattices is given in Sec. IV B. Brief discussions of polychromaticity in the context of bond percolation and of possible applications are presented in Secs. IV C and IV D. Section V contains a summary of the main points of the paper.

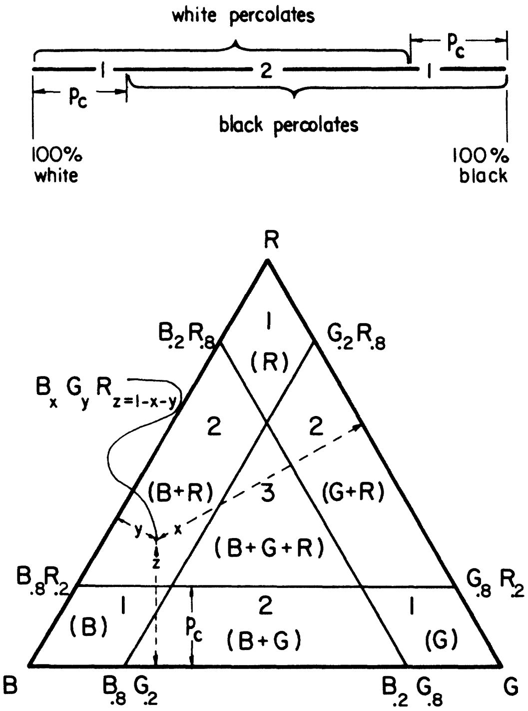

FIG. 1. Composition fields for site-percolation processes on the fcc lattice. The upper diagram corresponds to ordinary (black-and-white) percolation; the lower diagram corresponds to polychromatic percolalation with three colors (labeled blue, green, and red) present.

II. POLYCHROMATIC PERCOLATION

A. Coexisting percolating species

The familiar version of percolation is essentially a bichromatic process, although our attention is normally focused on the finite clusters and the presence or absence of a percolation path (infinite cluster) of just one of the two species present: the filled sites in site-percolation processes or the unblocked bonds in bond-percolation processes. A similar percolation problem exists for the other species present (the empty sites, or the blocked bonds), which is normally ignored. The composition of the system is determined by the single independent variable p, the fraction or concentration of the "species of interest." The complementary concentration of the "uninteresting" species is just $1-p$.

Since the composition diagram of an ordinary percolation system is one-dimensional, it can be represented by a line segment as at the top of Fig. 1. In this figure, the value of p_c corresponds to that for site percolation on the face-centered-cubic (fcc) lattice in three dimensions. (Each lattice treated, until Sec. IV, will be of the simple type with no bonds beyond nearest neighbors.) In order to emphasize the inherent symmetry between the two nongeometric states assigned to the sites, the composition line has been labeled in terms of the fractions of "black" and "white" sites rather than filled and empty sites. Since p_c is close to 0.2 in this case,[13] each individual species percolates over about 80% of the composition field, and *both* percolate in the central 60% of the field.

If, instead of just two colors present there are C colors, then there are C equivalent percolation problems. Consider $C=3$. For three-color site percolation, each site can be singly occupied by, say, either blue, green, or red "particles." Two adjacent sites of the same color (i.e., occupied by particles of the same color) are regarded as linked. For bond percolation, each bond is permeable to either the blue or the green or the red "fluid," and adjacent bonds of (permeable to the fluid of) the same color are linked.

With three colors present, two concentrations are needed to specify the composition. The two-dimensional composition diagram is the equilateral triangle familiar from the chemistry of ternary alloys, in which the vertices represent the pure elements, the edges represent the binary alloys, and the interior points (exploiting the invariance of the sum of the normals to the sides) represent all possible ternary compositions. Trichromatic site percolation on the fcc lattice is represented in this way on the lower part of Fig. 1. Each of the three lines which cut through the field corresponds to the locus of ternary compositions for which one component is present in a concentration equal to the percolation threshold. These loci symmetrically divide the composition field into regions in which various colors percolate. For the fcc lattice, which corresponds to close packing and is thus the most highly connected ($z = 12$) simple lattice in three dimensions, all three types of particles present in a three-color site-percolation process may simultaneously percolate (form infinite clusters) over about one-sixth of the composition field.

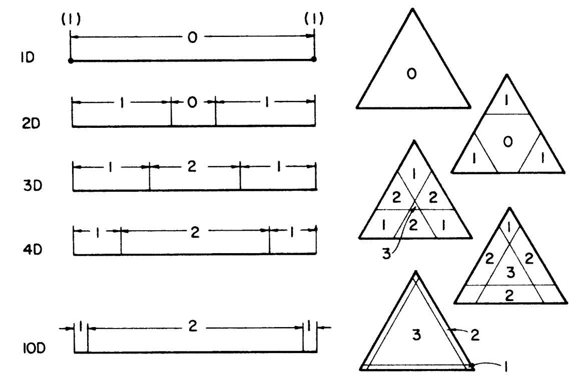

FIG. 2. Growth of panchromatic percolation with dimensionality (via increasing connectivity) for site percolation on d-dimensional simple cubic lattices. Two-color composition fields are on the left, three-color fields are on the right, and dimensionality increases from top to bottom ($d = 1$, 2, 3, 4, and 10).

B. Chromatic composition fields: $C = 2$, 3, and 4

Composition diagrams such as those in Fig. 1 provide a convenient characterization of the possibilities which can arise in a polychromatic percolation process. With C colors present, there are $C - 1$ independent concentrations x_i. We will use $C_p = C_p(x_i)$ to denote the number of percolating colors (number of i's for which $x_i > p_c$) at each composition (x_i). The boundaries of the composition regions of constant C_p are the loci $x_i = p_c$ (two points, three lines, or four planes, respectively, for $C = 2$, 3, or 4). The nature of the partition of the composition field by these loci depends on the relationship between C and p_c. If $p_c < C^{-1}$, there is a central region in which $x_i > p_c$ for all i so that *all* of the colors percolate. This situation obtains for both cases diagramed in Fig. 1. We will refer to a composition region in which $C_p = C$ as a *panchromatic regime*. If $p_c > C^{-1}$, there is a central region in which *none* of the colors percolate, i.e., a *nonpercolating regime* ($C_p = 0$).

To illustrate these two mutually exclusive situations and their variation with p_c (for constant C) we show in Fig. 2 the division of the two-color and three-color fields for site percolation on simple cubic (sc) lattices in 1, 2, 3, 4, and 10 dimensions. Percolation thresholds for site percolation on sc lattices in higher dimensions have been estimated through $d = 6$ by Kirkpatrick[10] using computer studies, and by Gaunt *et al.*[11] using series expansions. For the $d = 10$ sc lattice, the p_c used in the bottom row of Fig. 2 was estimated from their data by a simple extrapolation described in Sec. III A. In the one-dimensional case illustrated in the top row of Fig. 2, there is no percolation anywhere except at the singular (and singularly uninteresting) points corresponding to all sites being of one color. In two dimensions p_c is about 0.6,[11,14] so that the central part of the composition field is nonpercolating for both $C = 2$ and $C = 3$. In three dimensions, p_c is about 0.3,[10,13] and now the central region exhibits panchromatic percolation in both cases. With increasing dimensionality and a fixed number of colors, the panchromatic regime appears when p_c has dropped below C^{-1} and then grows to dominate the composition field (as has happened by $d = 10$ in Fig. 2).

When $C = 4$ the composition figure is a tetrahedron, and is dissected into at most 15 three-dimensional regions by the four $x_i = p_c$ planes. For the fcc lattice, each face of the tetrahedron is divided in the same way as is the three-color field of Fig. 1, while for the sc lattice each face is equivalent to the $C = 3$ diagram in the middle of the right side of Fig. 2. For both lattices, the four-color field contains a central region which does not intersect the faces of the tetrahedron. This interior region (which symmetrically surrounds the body center) is nonpercolating ($C_p = 0$) for the sc lattice, while for the fcc lattice it is a panchromatic regime ($C_p = 4$).

The following connection to an analogy alluded to in the Introduction is worth noting here. Each chromatic composition field (like the examples shown in Figs. 1 and 2, and the tetrahedra discussed above) is a figure which, *with the colors included*, exhibits a symmetry corresponding to a Belov point group.[12] In such a group, each geometric rotation or reflection acts in concert with a color-exchange operation.

In order to more quantitatively characterize the composition figure for polychromatic percolation, we introduce a set of quantities symbolized by

TABLE I. Polychromatic percolation with two, three, or four colors present. $F(C_p, C; p_c)$ is the fraction of the C-chromatic composition field over which C_p colors percolate, for a critical percolation threshold p_c. The bottom section lists some general relations in terms of C_0, the maximum C_p consistent with a given p_c. C_0 is the integer which satisfies $p_c^{-1} - 1 \le C_0 < p_c^{-1}$.

$C=2,\ p_c<\frac{1}{2}$	$C=2,\ p_c>\frac{1}{2}$	$C=3,\ p_c>\frac{1}{2}$	$C=C,\ p_c>\frac{1}{2}$
$F(0,2)=0$	$F(0,2)=2p_c-1$	$F(0,3)=1-3(1-p_c)^2$	$F(0,C)=1-F(1,C)$
$F(1,2)=2p_c$	$F(1,2)=2(1-p_c)$	$F(1,3)=3(1-p_c)^2$	$F(1,C)=C(1-p_c)^{C-1}$
$F(2,2)=1-2p_c$	$F(2,2)=0$	$F(2,3)=F(3,3)=0$	$F(C_p\ge 2, C)=0$

$C=3,\ p_c<\frac{1}{3}$	$C=3,\ \frac{1}{3}<p_c<\frac{1}{2}$
$F(0,3)=0$	$F(0,3)=(3p_c-1)^2$
$F(1,3)=6p_c^2$	$F(1,3)=3(1-p_c)^2-6(1-2p_c)^2$
$F(2,3)=3(1-2p_c)^2-3(1-3p_c)^2$	$F(2,3)=3(1-2p_c)^2$
$F(3,3)=(1-3p_c)^2$	$F(3,3)=0$

$C=4,\ p_c<\frac{1}{4}$	$C=4,\ \frac{1}{4}<p_c<\frac{1}{3}$
$F(0,4)=0$	$F(0,4)=(4p_c-1)^3$
$F(1,4)=24p_c^3$	$F(1,4)=24p_c^3-4(4p_c-1)^3$
$F(2,4)=6(1-2p_c)^3-12(1-3p_c)^3+6(1-4p_c)^3$	$F(2,4)=6(1-2p_c)^3-12(1-3p_c)^3$
$F(3,4)=4(1-3p_c)^3-4(1-4p_c)^3$	$F(3,4)=4(1-3p_c)^3$
$F(4,4)=(1-4p_c)^3$	$F(4,4)=0$

$C\le C_0$	$C>C_0$
$F(C,C)=(1-Cp_c)^{C-1}$	$F(C,C)=0, \quad F(0,C)\ne 0$
$F(0,C)=0$	$F(0,C_0+1)=[(C_0+1)p_c-1]^{C_0}<C_0^{-C_0}$
$F(C_0,C_0)=(1-C_0p_c)^{C_0-1}\le(C_0+1)^{-(C_0-1)}$	$F(C_0,C_0+1)=(C_0+1)(1-C_0p_c)^{C_0}\le F(C_0,C_0)$

$F(C_p, C; p_c)$. F is defined as the fraction of the C-chromatic composition field over which C_p colors percolate when the percolation threshold is p_c. Included in F are all of the $\binom{C}{C_p}$ symmetrically-related separate regions in which $x_i > p_c$ for exactly C_p colors and $x_i < p_c$ for the remaining $C - C_p$. For example, for site percolation on the fcc lattice, $F(2,3;0.198)$ is the fraction of the triangular field of Fig. 1 which is occupied by the three $C_p = 2$ trapezoids with their bases centered on the edges.

Expressions for $F(C_p, C; p_c)$ in terms of p_c for various C_p, C situations with $C=2$, 3, or 4, are straightforwardly obtained from an analysis of the geometry of composition figures like those discussed above. These are collected in Table I. As illustrations of these results, we show in Table II a numerical breakdown of the fractions corresponding to four-color site percolation on the three-dimensional sc and fcc lattices.[15] For the fcc case, multiple percolation ($C_p \ge 2$) occurs over more than 80% of the tetrahedral composition field.

TABLE II. Comparison of the composition fields for four-color site-percolation processes on the three-dimensional simple cubic (sc) and face-centered-cubic (fcc) lattices.

$F(C_p, C)$	sc; $p_c=0.311$	fcc; $p_c=0.198$
$F(0,4)$	1.5%	0.0%
$F(1,4)$	66.4%	18.6%
$F(2,4)$	32.0%	57.3%
$F(3,4)$	0.12%	23.2%
$F(4,4)$	0.0%	0.9%

C. Chromatic composition fields: $C>4$

In general, with C colors present, the composition figure is a $(C-1)$-dimensional *simplex*, i.e., the simplest polytope[16] (generalized polyhedron) in $C-1$ dimensions. Thus, with $C=5$, the figure is a pentatope, or five cell, in four dimensions. The partition of the simplex by the $x_i = p_c$ hyperplanes requires analysis of such higher-dimensional geometries for $C>4$. Although techniques exist for this,[16] we shall confine ourselves here to several important generalizations to large C which can be obtained directly or by induction. Most of these have been included in Table I.

The entries at the end of the top row in Table I reflect the fact that if the percolation threshold exceeds $\frac{1}{2}$, multiple percolation *cannot* occur and the field is divided between the nonpercolating region and C monopercolating regions:

$$\left.\begin{aligned} F(0,C) &= 1 - F(1,C), \\ F(1,C) &= C(1-p_c)^{C-1}, \\ F(C_p \geq 2, C) &= 0. \end{aligned}\right\} p_c > \tfrac{1}{2}. \quad \begin{aligned}(1a)\\(1b)\\(1c)\end{aligned}$$

The expression for $F(1,C)$ follows directly from the observation that the monopercolating region which adjoins each of the C vertices of the $(C-1)$-dimensional composition simplex is a similar simplex whose edge is reduced by a factor of $1-p_c$. Examples of this situation are the diagrams in the second row of Fig. 2, corresponding to $C=2$ and $C=3$ for site percolation on the square lattice.

More interesting than (1) are the general relations which make up the last row of Table I. These involve a special value C_0 for the number of colors. C_0 is the maximum number of colors which can simultaneously percolate for a given percolation threshold, i.e., it is the largest integer whose reciprocal (C^{-1} is the concentration of each color when all x_i are equal) exceeds p_c,

$$p_c^{-1} - 1 \leq C_0 < p_c^{-1}. \quad (2)$$

When the number of species is below C_0, or equal to it, the composition field contains a panchromatic regime and no nonpercolating regime:

$$\left.\begin{aligned} F(C,C;p_c) &= (1-Cp_c)^{C-1}, \\ F(0,C;p_c) &= 0. \end{aligned}\right\} C \leq C_0. \quad \begin{aligned}(3a)\\(3b)\end{aligned}$$

Equation (3a) for the panchromatic fraction can be arrived at by induction from the results in Table I for $F(C,C;p_c<C^{-1})$ with $C=2$, 3, and 4, as well as by observing that the panchromatic region is a simplex whose edge is reduced by a factor of $1-Cp_c$ with respect to that of the full simplex (e.g., the last three rows of Fig. 2). The behavior of $F(C,C)$ as a function of p_c, for several values of C, will be shown graphically in Sec. IV A. When $C=C_0$, (2) and (3a) yield the following upper bound for the panchromatic fraction:

$$F(C_0,C_0) \leq (C_0+1)^{-(C_0-1)}. \quad (4)$$

When $C>C_0$, there is a nonpercolating regime and no panchromatic regime. No simple general expression analogous to (3a) can be written down for the nonpercolating fraction because, for a given C, the nonpercolating region intersects the simplex boundaries and changes shape $C-2$ times as p_c is increased from C^{-1} to 1. For the specific case $C=C_0+1$, expressions for $F(0,C_0+1)$ and $F(C_0,C_0+1)$, as well as upper bounds analogous to (4), are given in Table I.

Several other results for general C, such as

$$F(1,C;p_c<C^{-1}) = Cp_c^{C-1}, \quad C<C_0 \quad (5)$$

for the monochromatic-percolation fraction when at least one must percolate, are readily apparent via induction from Table I.

III. PERCOLATION IN HIGHER DIMENSIONS

A. Critical volume fraction

The construct of a critical volume fraction[17] for percolation processes has proven useful in a variety of applications to microscopically[5,7] and macroscopically[18] heterogeneous solids composed of conducting and insulating regions. The critical volume fraction $\phi_c(d)$ is defined as $\langle p_c^j(d) f_j(d)\rangle$, where $p_c^j(d)$ is the site-percolation threshold for the simple (nearest-neighbor bonds only) lattice j in d dimensions. Here, $f_j(d)$ is the filling factor of the lattice corresponding to the packing of equal touching nonoverlapping d-dimensional spheres centered on the lattice sites. The utility of $\phi_c(d)$ in two and three dimensions is based on the empirical rule that, while p_c^j varies strongly with j, the product $p_c^j f_j$ (corresponding to the fraction of space which, at the site-percolation threshold, is occupied by the spheres containing filled sites) is nearly *independent* of j for given d.[17] Thus, at least for $d=2$ and $d=3$, $p_c^j f_j$ is a "dimensional invariant" (a form of "universality") which depends on dimensionality but does *not* depend on the details of lattice geometry:

$$p_c^j(d) f_j(d) \approx \phi_c(d). \quad (6)$$

While the values of p_c for site percolation on the three-dimensional fcc, sc, body-center-cubic, and diamond-structure lattices vary between 0.198 and 0.428,[13] the values of $p_c^j f_j$ for all four fall within the range 0.156 ± 0.010.

If (6) were to be valid for $d>3$ as it is for $d=2$ and $d=3$, it would provide a painless method for obtaining a quick estimate of p_c for site percolation on a d-dimensional lattice, based on a known p_c for some other lattice of the same dimensionality. From the work of Kirkpatrick[10] and of Gaunt *et al.*,[11] p_c is known for higher-dimensional sc lattices (hypercubic lattices) through $d=6$. Their results for $d=4$, 5, and 6 are well fit by

$$p_c^{sc} \approx (1+6.3d^{-2})(z_{sc}-1)^{-1}, \quad d \geq 4 \quad (7)$$

where $z_{sc}=2d$ is the coordination number. Because of the rapid approach (in the sc case) to the Bethe-lattice (BL) limit $(z-1)^{-1}$, Eq. (7) can be used to obtain good estimates for higher d. Since $p_c^{sc}(d)$ is now closely known for all d, the validity of (6) in d dimensions would allow us to approximate $p_c^j(d)$, for any lattice j, simply by $p_c^{sc}(d) f_{sc}(d)/f_j(d)$.

Unhappily, the above prescription does not work for d sufficiently large. This can be demonstrated as follows. Suppose that, in d dimensions, we compare the sc lattice to the lattice which is the generalization of the fcc lattice. In four dimensions, for example, Cartesian coordinates for the nearest-neighbor sites of a site at the origin would be of the form (±1, 0, 0, 0) for the sc lattice (with eight nearest neighbors) and (±1, ±1, 0, 0) for the fcc lattice (with 24 nearest neighbors). In general, $z_{sc}(d) = 2d$ and

$$z_{fcc}(d) = 4\binom{d}{2} = 2d^2 - 2d\,. \tag{8}$$

It is not hard to show that the filling factors for the two lattices are given by

$$f_{sc}(d) = 2^{-d}v(d)\,, \tag{9a}$$

$$f_{fcc}(d) = 2^{-(d/2)-1}v(d)\,, \tag{9b}$$

where $v(d)$ is $\pi^{d/2}/\Gamma(\frac{1}{2}d+1)$, the volume of the d-dimensional sphere of unit radius. If (6) could now be used, then the following expression for $p_c^{fcc}(d)$ could be obtained by combining (6), (7), and (9):

$$2^{-(d/2)+1}(1+6.3d^{-2})(2d-1)^{-1}\,. \tag{10}$$

However, p_c must exceed[2] the BL value $(z-1)^{-1}$, so that, using (8)

$$p_c^{fcc}(d) > (2d^2 - 2d - 1)^{-1}\,. \tag{11}$$

For $d \geq 9$, the "estimate" given in (10) falls below, and therefore violates, the lower bound given in (11).

Thus the idea of lattice-independent dimensional-invariant critical volume fraction $\phi_c(d)$ cannot be extended indefinitely; it fails for dimensions of nine or more. Because (6) does work so well in two and three dimensions, we shall assume that the failure sets in smoothly and that ϕ_c remains a useful approximation in four and five dimensions. This assumption is supported, as described below, by results obtained in Sec. III B. Using the p_c^{sc} and f_{sc} values of Table III and Eq. (9a), we obtain the estimates

$$\phi_c(d=4) = 0.061\,, \tag{12a}$$

$$\phi_c(d=5) = 0.023\,. \tag{12b}$$

Estimates based on (12) are obtained for $p_c^{fcc}(d=4)$ and $p_c^{fcc}(d=5)$ in Sec. III B. These are found to agree well with other estimates discussed below, providing evidence for the utility of (6) for dimensionalities up to $d=5$.

B. Close-packed lattices in d dimensions

Close-packed (cp) lattices in higher dimensions provide examples of lattices of very high connectivity. However, until now, no estimates have been given for $p_c^{cp}(d)$ for $d>3$. In this section, we induce estimates (which, although rough, provide the only such values thus far available) for site-percolation thresholds for cp lattices in d from 4 to 8.

Quantities relevant to polychromatic percolation on cp lattices are listed in Table III, along with some corresponding values for sc lattices. The coordination number $z_{cp}(d)$ for close packing is known up to $d=8$.[19] For $d=2$, p_c^{cp} is $\frac{1}{2}$ (the exact result known for site percolation on the triangular lattice[20]) and for $d=3$, p_c^{cp} is 0.198.[13] The bracketed values in column 8 of Table III are our estimates for p_c^{cp} for $d=4-8$. Each of these is an average of separate estimates given in columns 9–11. Column 9 shows the values based on the critical volume fractions of Eq. (12). Column 10 is based on the observation that the amount by which the BL limit $(z-1)^{-1}$ underestimates the site-percolation threshold is nearly the same (0.10 ± 0.01) for different three-dimensional lat-

TABLE III. Quantities relevant to polychromatic percolation for site-percolation processes on simple cubic and close-packed lattices in d dimensions. z is the lattice coordination number, p_c is the site-percolation threshold, and C_0 is the maximum number of percolating colors. ϕ_c is the critical volume fraction, a dimensional invariant useful for $d=1$–5. Bracketed values for p_c are estimates based on the extrapolations shown in succeeding columns.

	Simple cubic lattices					Close-packed lattices					
d	ϕ_c	z_{sc}	p_c^{sc}	$(1+6.3d^{-2}) \times (z_{sc}-1)^{-1}$	C_0^{sc}	z_{cp}	p_c^{cp}	ϕ_c/f_{cp}	$p_c^{sc}-(z_{sc}-1)^{-1} + (z_{cp}-1)^{-1}$	$2.2 \times (z_{cp}-1)^{-1}$	C_0^{cp}
1	1.00	2	1.000		0	2	1.000	1.00	1.00		0
2	0.45	4	0.593 [a]		1	6	0.500 [b]	0.50	0.46	0.44	1
3	0.156	6	0.311 [c]		3	12	0.198 [d]	0.21	0.20	0.20	5
4	0.061	8	0.198 [e]	0.199	5	24 [f]	[0.098]	0.099	0.099	0.096	10
5	0.023	10	0.141 [e]	0.139	7	40 [f]	[0.054]	0.050	0.056	0.056	18 ± 1
6		12	0.107 [e]	0.107	9	72 [f]	[0.031]		0.030	0.031	32 ± 2
7		14	[0.087]	0.087	11	126 [f]	[0.018]		0.018	0.018	55 ± 6
8		16	[0.073]	0.073	13	240 [f]	[0.010]		0.011	0.009	100 ± 20

[a] Reference 14.
[b] Reference 20.
[c] References 10 and 13.
[d] Reference 13.
[e] References 10 and 11.
[f] Reference 19.

tices. Assuming the same for $d>3$, these estimates are obtained from $z_{cp}(d)$ and the known $p_c^{sc}(d)$ values by setting $p_c^{cp}-(z_{cp}-1)^{-1}$ equal to $p_c^{sc}-(z_{sc}-1)^{-1}$.

These two methods for estimating $p_c^{cp}(d)$ yield values in good agreement with the known values for $d=1-3$, and with each other for $d=1-5$. For sc lattices, which in high dimensions are lattices of relatively *low* connectivity, we noted in Sec. III A that p_c^{sc} rapidly converges to the BL limit $(z_{sc}-1)^{-1}$ with increasing d. *This does not happen for the close-packed lattices.* The ratio of p_c^{cp} to $(z_{cp}-1)^{-1}$ for $d=2$, 3, 4, and 5 is 2.5, 2.2, 2.3, and 2.1 (using the above estimates for the last two). For cp lattices, the approach of the site-percolation threshold to the Bethe-lattice limit with increasing d, *if it occurs at all*, is painfully slow. Assuming little progress in the approach (to the BL limit) by $d=8$, we include values of $2.2(z_{cp}-1)^{-1}$ in column 11 of Table III as another approximation for p_c^{cp}.

The behavior of z, p_c, and C_0 for cp and sc lattices is shown in Fig. 3. (Also included is ϕ_c, which gradually drops away from p_c^{cp} as the filling factor for close packing falls from 1 at $d=1$ to 0.465 at $d=5$). The dimensionality dependence of each of these quantities is much stronger for cp than for sc lattices.

From three dimensions up to eight, the quantities for cp lattices can be approximated by exponentials with a geometric ratio of 1.8:

$$\left.\begin{aligned} z_{cp}(d) &\approx 2.17\times(1.8)^d, \quad &(13a)\\ p_c^{cp}(d) &\approx 1.10\times(1.8)^{-d}, \quad &(13b)\\ C_0^{cp}(d) &\approx 0.91\times(1.8)^d, \quad &(13c)\end{aligned}\right\}\; 3\leq d\leq 8 .$$

Equation (13a) can be compared with an asymptotic upper limit derived by Coxeter[19]:

$$z_{cp}(d)<(\pi/2)^{1/2}e^{-1}d^{3/2}2^{d/2}, \quad d\to\infty . \tag{14}$$

This asymptotic upper bound approaches a geometric progression of ratio $\sqrt{2}$.

The reciprocal relation between (13b) and (13c) simply reflects the fact that, because p_c is so small, C_0 is essentially p_c^{-1} for highly connected lattices. However, the threshold-versus-connectivity relation between (13a) and (13b) is extremely interesting:

$$p_c^{cp}(d)z_{cp}(d)\approx 2.4, \quad 3\leq d\leq 8 . \tag{15}$$

This relation for close packing, which cuts across *different dimensionalities*, is reminiscent of an asymptotic limit which Domb and Dalton[21] obtained for site percolation on highly connected complex lattices (with bonds beyond nearest neighbors) of the *same* dimensionality. The connection between

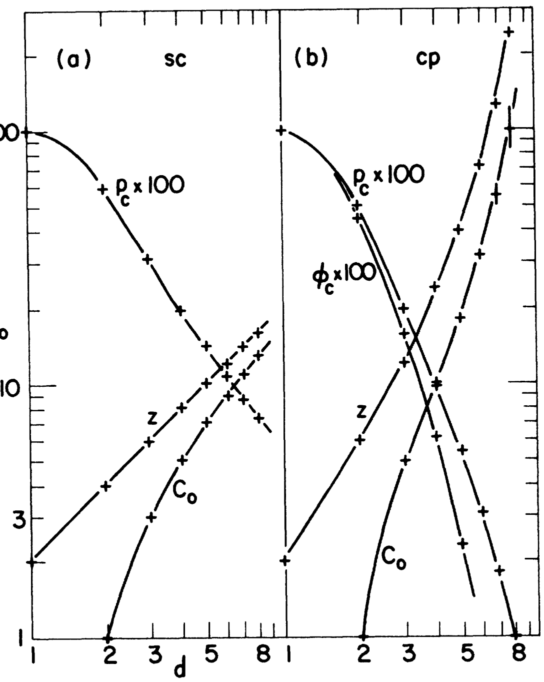

FIG. 3. Site-percolation threshold p_c, coordination number z, and maximum number of simultaneously percolating species C_0, shown as a function of d for d-dimensional simple cubic (a) and close packed (b) lattices. Included in (b) is the lattice-independent critical volume fraction ϕ.

(15) and the result of Domb and Dalton is given in Sec. IV B.

IV. THE COEXISTENCE OF UNBOUNDED CLUSTERS IN HIGHLY CONNECTED LATTICES

A. Polychromatic percolation in higher dimensions

We now exhibit the consequences for polychromatic percolation of the dimensionality dependences of Fig. 3. Thus far only C_0, the maximum possible number of percolating species, has been given as a function of d. C_0 is an oversimplified measure of the connectivity-enhanced opportunities for multiple percolation. It can also be misleading in that, for high connectivity and large C_0, it exaggerates the possibilities. Inequality (4) of Sec. II C reveals that when C_0 is large, the regime in which C_0 colors percolate with C_0 colors present occupies only a minute fraction of the composition field.

Much more complete information is contained in the full set of numbers $F(C_p, C)$ which specify the fraction over which C_p out of C species percolate. Even if we restrict ourselves to the finite subset of cases with $C_p\leq C\leq C_0$, there are $\frac{1}{2}(C_0^2+C_0)$ nonvanishing F's to contend with, which rapidly be-

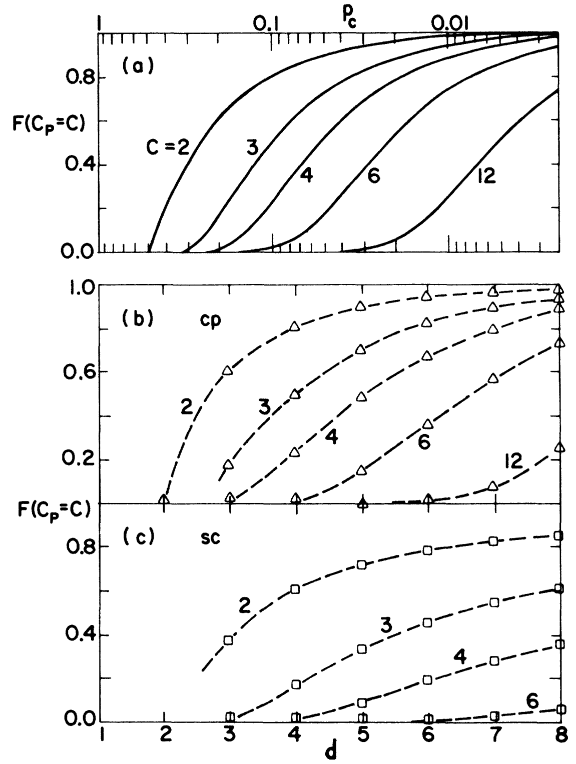

FIG. 4. Panchromatic percolation fraction with 2, 3, 4, 6, or 12 colors present. $F(C,C;\,p_c)$ is shown in (a) as a function of the percolation threshold for a site or bond process on a general lattice, and also as a function of d for site percolation on the d-dimensional close-packed (b) and simple cubic (c) lattices discussed in the text.

comes cumbersome. Besides which, explicit expressions for $F(C_p, C; p_c)$ are not available for all general cases with $C>5$. However, the general expression for the panchromatic fraction $F(C_p=C)$ was obtained [as Eq. (3a)] in Sec. II C. This quantity, evaluated for various values of C smaller than C_0, provides a fine measure of the scope for multiple percolation.

Figure 4(a) displays the panchromatic fraction as a function of the percolation threshold with 2, 3, 4, 6, or 12 colors present. The p_c scale is exponential, extending from unity down to below 3×10^{-3}. Increasing the number of colors not only shifts the onset of panchromaticity to lower p_c, it also makes the onset progressively softer.

Using the information of Fig. 3, we present analogous results for site percolation in higher-dimensional lattices in Figs. 4(b) (for cp lattices) and 4(c) (for sc lattices), plotted this time against d from 1 to 8. The rapid growth of panchromaticity for cp lattices, and the relative sluggishness for sc lattices, is clearly seen. With $d=8$, the panchromatic regime for $C=6$ dominates the field for the cp lattice, but is barely appreciable for the sc lattice. Similarly, $F(C_p=C)$ for $C=2$, 3, and 4 have all approached closer to saturation (at $d=8$) for the cp lattice than has $C=2$ for the sc lattice.

B. Highly connected lattices in two and three dimensions

The basic requirement for polychromatic percolation is simply a low threshold, as shown in Fig. 4(a). Thus far we have used higher-dimensional nearest-neighbor-connected lattices to illustrate the effects of decreasing p_c within a given lattice type. By dropping the limitation to simple lattices with bonds only between nearest-neighbor sites, and adding connections *beyond* nearest neighbors, we can encounter quite low thresholds in three dimensions and even in two.

Domb and Dalton[21] determined p_c for several two- and three-dimensional lattices in the presence of such longer-range interactions. For the triangular lattice (cp lattice for $d=2$), the addition of connections out to third-nearest neighbors raises z to 18 and lowers p_c to 0.22. Thus the ability for two sites of the same color to communicate in spite of intervening sites of other colors introduces the possibility of polychromatic percolation into two-dimensional site-percolation processes. In three dimensions, the addition of bonds out to third neighbors raises z to 26 and lowers p_c to 0.10 for the sc lattice, while the fcc lattice achieves a coordination number of 42 and a site-percolation threshold of 0.06. By further increasing the range, z can be made arbitrarily large and p_c arbitrarily small.

The indicated correspondence between the effect of increasing dimensionality (for fixed range) and of increasing range (for fixed dimensionality) can be epitomized in a few remarkably simple empirical correlations. The product $p_c z$ states the average number of filled sites accessible to a given site at the percolation threshold. In Eq. (15) we noted that for d-dimensional close-packed lattices, this product is approximately *independent of dimensionality* (with a value of 2.4) for $d\geq3$. Domb and Dalton[21] noted relations analogous to this one for site percolation on various lattices *of the same dimensionality* as they increased the range. They observed that $p_c z$ approached 4.5 in two dimensions, 2.7 in three dimensions. Since z is so large for the close-packed lattices in higher dimensions, our result clearly suggests that the limiting value at high dimensionality of the isodimensional asymptotic limit ($z\to\infty$ at constant d) of Domb and Dalton is 2.4.

C. Bond percolation

All of the specific cases treated here have dealt with site percolation, but it is important to recognize the applicability to bond-percolation processes as well. Thus Fig. 4(a), as well as Table I, applies to both bond and site processes. In fact, a moment's thought reveals that we have been somewhat conservative in focusing on site processes since on any given lattice, $p_c(\text{bond}) < p_c(\text{site})$[1,2] (except for a Bethe lattice, where the two coincide). From Table II, we know that for four-color site percolation on the $d=3$ fcc lattice (with $p_c = 0.198$), the panchromatic regime occupies less than 1% of the composition tetrahedron. For the corresponding bond-percolation process (with $p_c = 0.12$) the panchromatic regime is far more extensive, occupying 14% of the field.

The most striking example of the greater generosity which bond processes display toward multiple percolation is the nearest-neighbor-connected triangular lattice. As with all other simple two-dimensional lattices, polychromatic percolation is *not* possible for site percolation on this lattice (p_c is $\frac{1}{2}$ and C_0 is 1). For bond percolation, however, p_c is 0.347 for the triangular lattice,[20] so that two colors *can* simultaneously percolate. The reason that a pair of unbounded two-dimensional clusters (infinite "spider webs") can interpenetrate each other in the bond-percolation case is that the two spider webs are permitted to cross each other at the sites. No such crossing is allowed in the nearest-neighbor site-percolation case, so that the existence of one extended web precludes the occurrence of a second.[22]

D. Possible applications

One possible application of these ideas in a bond-percolation context is the question of extended propagation of multiple signals on a communications network composed of saturable lines. A site-percolation example would be a substitutional mixed crystal in which each atom can communicate only with other atoms of the same type. Exciton motion in molecular crystals is a candidate here, since the resonance-transfer mechanism for energy migration requires chemical identity between the transmitting and receiving molecules. Conventional percolation has recently been applied to exciton transfer processes,[23] and polychromatic percolation could provide a model for exciton motion within *several* of the chemically distinct sublattices which make up a substitutionally disordered mixed-crystal system. Multiple percolation could be favored in such a system because the resonance-transfer interaction extends well beyond nearest neighbors, so that the lattice is effectively highly connected.

For composite materials made up of a number of different solid phases, an important and difficult problem is the estimation of bulk properties of the composite from the properties of the components. Recent studies[24] of calculational techniques for multicomponent media indicate that results depend on which phases are percolating and which are not. The critical fraction $\phi_c(d=3)$ would replace p_c in the construction of the chromatic composition figure for such a case.

V. SUMMARY

We have developed a generalization of percolation from a two-species black-and-white process to a multispecies, polychromatic process. The partition of the C-chromatic composition field, a key characteristic of polychromatic percolation (Figs. 1 and 2), has been analyzed via the quantities $F(C_p, C; p_c)$ defined in Sec. II. The general result [Eq. (3a)] for the fraction of the field occupied by the panchromatic regime provides a useful measure of the scope for multiple percolation, and has been shown as a function of p_c in Fig. 4(a) for $C = 2$, 3, 4, 6 and 12.

Polychromatic percolation is richest for highly connected lattices, in which many species can simultaneously percolate. As examples of high-connectivity low-p_c lattices, we have considered site-percolation processes on d-dimensional simple cubic and close-packed lattices, as well as a few two- and three-dimensional lattices with long-range interactions. The growth of polychromaticity with dimensionality for sc and cp lattices has been demonstrated in Fig. 4.

Higher dimensions have entered in two ways: in Sec. II C as the dimensionality of composition fields for $C > 4$, and in Secs. III and IV A dealing with d-dimensional lattices as examples of high connectivity. Estimates have been obtained, for the first time, for p_c for site percolation on close-packed lattices for d from 4 to 8 (Fig. 3). For cp lattices the product $p_c z$ is approximately 2.4 for $d \geq 3$, a remarkably simple result analogous to Domb and Dalton's asymptotic limits for high z at constant d. Also, the concept of a lattice-independent dimensional-invariant critical volume fraction for site percolation has been extended to $d=4$ and 5, although it is shown to ultimately fail for $d > 8$.

Finally, polychromatic percolation has been briefly discussed in the context of bond percolation and of possible applications. Many avenues exist for extending these ideas, such as permitting the species in site processes to have different interaction ranges (and thereby different p_c's). Only the simplest cases have been considered here.

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