Critical Percolation Probabilities (Site Problem)

H. L. FRISCH, E. SONNENBLICK, AND V. A. VYSSOTSKY
Bell Telephone Laboratories, Murray Hill, New Jersey

AND

J. M. HAMMERSLEY
University of Oxford, Oxford, England

(Received July 7, 1961)

Monte Carlo estimates of the critical percolation probabilities for the "site problem" are presented for a number of two- and three-dimensional crystal lattices. The connection with the critical concentration of magnetic elements of certain models of random (magnetically dilute) ferromagnetic crystals is noted.

IN a previous publication,[1] we defined two percolation problems of physical interest, the "bond problem" and the "site problem," and gave numerical estimates of the critical probability for the "bond problem" $p_c(B)$ for a number of two- and three-dimensional crystal lattices. Here we shall present numerical estimates of the critical probability for the "site problem" $p_c(S)$ for the same crystal lattices as used in the previous study.[1] We shall display our results in Table I in a form convenient for comparison with estimates of $p_c(S)$ obtained from series expansions for the mean cluster size.[2–4] The probability $p_c(S)$ is the limiting concentration of magnetic elements, in a random (magnetically dilute) Heisenberg or Ising model of a ferromagnetic crystal, below which there is no Curie temperature.[3,4]

A modification of the previously used[1] Monte Carlo procedure, adapted for an IBM 7090 computer, was developed for numerically estimating the $p_c(S)$. We present in Table I the mean critical probabilities in 100 runs in which finally N vertices are "wetted" by the percolating "fluid." In this study N is either 1000 or 2000. For the three three-dimensional lattices for which the coordination number z exceeded 4, the storage capacity was quickly exceeded above $N=1000$ and thus we are unable to give results in these cases for $N=2000$. The average machine computation time per run is about 0.006 hr if $N=2000$. The value of p_c shown in Table I (plus or minus the standard deviation) is the sample mean for those runs in which a higher p was required to "wet" 2000 or 1000 vertices than to "wet" 100 vertices.

We note first that in those cases for which Monte Carlo estimates are available for both $N=1000$ and $N=2000$ vertices "wetted" that these agree well within the standard deviation for the mean. From Fig. 1 we see that if $p(S,n)$ represents the expected probability of site occupation at which n vertices have been "wetted" then $p(S,n)$ appears to approach $p_c(S)$ exponentially with n. This is similar to the behavior of the numerical results for the "bond problem."[1] Both the agreement in the entries of Table I and the form of the curves of Fig. 1 suggest that some confidence can be placed in the accuracy of the estimate of the mean critical probability on "wetting" only 1000 vertices.

A number of tests of the self-consistency of the numerical data, suggested by theory, can be applied: (1) In all instances $p_c(S)>p_c(B)$; it is known that $p_c(S)\geq p_c(B)$.[5] (2) In accord with theory[6] $p_c(S)$ for the plane square lattice is larger than (or equal to) $\frac{1}{2}$. (3) In accord with theory[5] the sum of $p_c(S)$ for the plane hexagonal and triangular lattices is larger than (or equal to) 1.

The Monte Carlo estimates of $p_c(S)$ and the estimates obtained by Domb and Sykes[2] and Rushbrooke and Morgan[4] (at least for the three-dimensional lattices) agree fairly satisfactorily, although the former are uniformly about 5–10% higher than the latter. We note again that $p_c(S)$, like $p_c(B)$,[1] in all cases listed in Table I appears to be little affected by differences of lattice type if the number of dimensions and coordination number are the same. The probabilities $p_c(S)$, like $p_c(B)$,[1] increase with decreasing z, for fixed d, in all cases cited in Table I. This increase of the critical

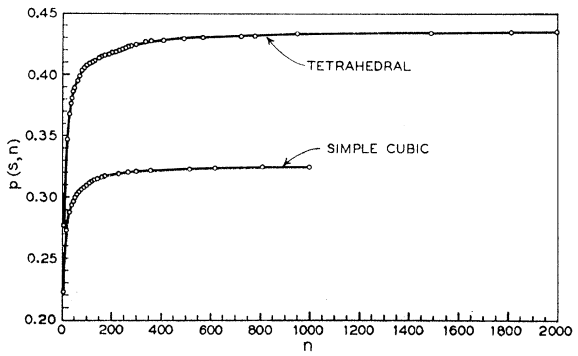

FIG. 1. Plot of $p(S,n)$ vs n for the simple cubic and tetrahedral lattices. Other lattice structures give a curve analogous to these.

[1] V. A. Vyssotsky, S. B. Gordon, H. L. Frisch, and J. M. Hammersley, Phys. Rev. **123**, 1566 (1961).
[2] C. Domb and M. F. Sykes, Phys. Rev. **122**, 77 (1961).
[3] R. J. Elliott, B. R. Heap, D. J. Morgan, and G. S. Rushbrooke, Phys. Rev. Letters **5**, 366 (1960).
[4] G. S. Rushbrooke and D. J. Morgan, Mol. Phys. **4**, 1 (1961).
[5] J. M. Hammersley, J. Math. Phys. **2**, 728 (1961).
[6] M. E. Fisher, J. Math. Phys. **2**, 620 (1961).

TABLE I. Critical probabilities (with d number of dimensions and z the coordination number of the lattice).

Lattice	d	z	$p_c(S)$ $N=1000$	$p_c(S)$ $N=2000$	$p_c(S)$ (ref. 2)	$p_c(S)$ (ref. 3)	$p_c(S)$ (ref. 4)	$p_c(B)$ $N=2000$ (ref. 1)
Triangular	2	6	0.487±0.021	0.493±0.018	0.51	0.36	···	0.341±0.011
Square	2	4	0.575±0.017	0.581±0.015	0.55	0.48	0.48	0.493±0.013
Hexagonal	2	3	0.683±0.020	0.688±0.017	$0.6<p_c<0.75$	0.49	···	0.640±0.018
hcp	3	12	0.204±0.008	···	···	···	···	0.124±0.005
fcc	3	12	0.199±0.008	···	···	···	0.18	0.125±0.005
Simple cubic	3	6	0.325±0.023	···	0.28	···	0.28	0.254±0.013
Tetrahedral	3	4	0.434±0.013	0.436±0.012	···	···	···	0.390±0.011
Ice (quartz)	3	4	0.432±0.013	0.433±0.011	···	···	···	0.388±0.010

probability with decreasing z is less rapid for the "site problem" than for the "bond problem." A number of simple algebraic relations between $p_c(S)$, z, and d can be found which reproduce about equally satisfactorily the numerical data in Table I. However, unless the class of lattices under consideration is restricted (e.g., to regular tessellation lattices), counterexamples to the simplest such relations are easily obtained. For example, if we let p denote $p_c(S)$ for the plane hexagonal lattice, and let $\tilde{p}$ denote $p_c(S)$ for the lattice of Fig. 2, it is easily seen that

$$p\leq\tilde{p}[1-(1-\tilde{p})^3],$$

so $p<\tilde{p}$, although both lattices have $z=3$. Likewise, if p' and $\tilde{p}'$ stand for $p_c(B)$ for the plane hexagonal lattice and the lattice of Fig. 2, respectively, then clearly

$$p'\leq\tilde{p}'^2,$$

so again $p'<\tilde{p}'$. Gilbert has constructed plane lattices with $z=3$ which have similar properties, and, in addition, have both point symmetry and line symmetry.

As an internal check on the consistency of the computer programs, $p_c(S)$ and $p_c(B)$ were computed for a square lattice with all bonds doubled. Doubling the bonds should leave $p_c(S)$ unaltered, while substituting $1-[1-p_c(B)]^{\frac{1}{2}}$ for $p_c(B)$. Hence the results for the usual square lattice lead us to expect values for the square lattice with doubled bonds of about 0.575 for $p_c(S)$ and 0.288 for $p_c(B)$. The values actually determined by the computer programs are 0.580±0.016 and 0.287±0.009.

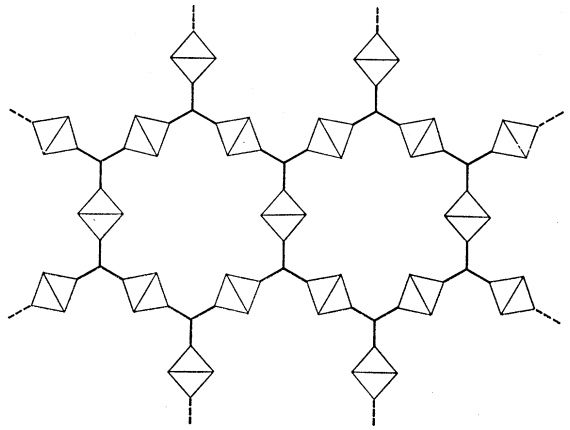

FIG. 2. Plane lattice with $z=3$. This lattice has values of $p_c(S)$ and $p_c(B)$ different from the values for the plane hexagonal lattice.