

Relations Between Site Percolation Thresholds

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By decomposing certain lattices into two sublattices, and examining at percolation threshold the structure of their infinite clusters, an approximate relation between p_c^0 , of the original lattice and p_c^I , of the sublattice is established: $p_c^0 \approx (p_c^I)^{1/2}$. It is conjectured that an inequality always holds: $p_c^0 \leq (p_c^I)^{1/2}$, and heuristic arguments are given to substantiate it. By similar considerations good estimates for p_c of certain correlated percolation problems are also obtained.

KEY WORDS: Percolation; critical concentration; decomposable lattice; sublattice; linking cluster.

1. INTRODUCTION

Much work has been done in the last few years in the field of percolation. Most of the modern work aims at calculation of the critical indices, looking for relations among them, and checking for universality hypotheses and looking for universality classes. Much less efforts were directed toward the more classical problem of finding the percolation thresholds and establishing relations among them. This is due perhaps to the fact that the natural parameter in the modern work is $p - p_c$, so that p_c itself does not play an essential role in the theory. In the present note an attempt is made to reveal relations among critical probabilities in some lattices for the site problem. These relations are essentially in the form of estimates: when the critical probability is given for a certain lattice (e.g., the triangular lattice) it is possible sometimes to estimate the value of the corresponding probability

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for another lattice (honeycomb in this example). It is also conjectured—with no solid proof as yet—that these relations may be formulated as inequalities, that is, the estimate (for the honeycomb) is in fact an upper bound for the actual threshold.

The present estimates are extremely simple and hardly involve any computation. It is therefore not surprising that with such a small amount of effort the results are exclusively limited to critical probabilities and not at all to indices. It should also be stressed that the method presented here is not universal, in the sense that it is not applicable to all systems but rather to a certain class, namely, to decomposable lattices only and their corresponding sublattices. Although decomposable lattices are discussed later, let us remark here that they appear in the theory of antiferromagnets as the lattices on which no frustration effects may be revealed. In Section 2 the notion of decomposable lattices is defined and the estimates, the approximation, as well as the conjecture are described and discussed in detail, and justified in a heuristic way for the uncorrelated problem. In Section 3 an application of the same method for a specific correlated problem is briefly described.

2. DECOMPOSABLE LATTICES

Let us look at the class of lattices in any number of dimensions which have the following property: If there is a loop on the lattice it contains an even number of sites. Examples of such lattices are the honeycomb (HC) and the square (S) lattices in two dimensions, the diamond (D), the simple cubic (SC) and the body-centered-cubic (BCC) lattices in three dimensions. Also Bethe lattices—of which the one-dimensional lattice is a degenerate example—of any coordination number belong to this class, as they do not have loops. This is also true for Bethe lattices with mixed coordination numbers. In all these lattices it is assumed that bonds exist only between nearest neighbors. Fairly simple and common lattices which do not belong to this class are the triangular (T) and Kagome lattices in two dimensions, the face-centered-cubic lattice (FCC) in three dimensions, and practically any lattice X , where both nearest and next nearest neighbors are directly connected [such a lattice is denoted by $X(1,2)$]. Any lattice in this class is decomposable in a unique way into two sublattices: if one site on the original lattice (this lattice will be denoted O) belongs to a sublattice I, then all its neighbors with which it is directly connected (or interact) on O by a bond belong to the second sublattice II, and vice versa. It is obvious that when all the sites on O are equivalent, the two sublattices are also equivalent. Two sites on one sublattice are connected by a bond (interact) if there is at least one site on the other sublattice which interacts with both on O .

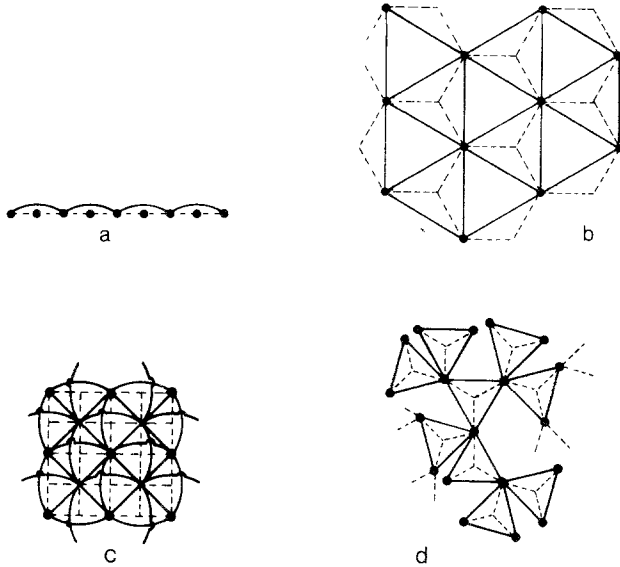


Fig. 1. Examples of some decomposable lattices θ (bonds denoted by dashed lines) and their corresponding sublattices (bonds denoted by solid lines). For each θ lattice only one of the sublattices is indicated. (a) Linear lattice. (b) Honeycomb and triangular. (c) Square and square (1, 2). (d) Bethe lattice with coordination number 3 and the corresponding cactus. The bonds between next nearest neighbors on the sublattice in (a) and (c) are drawn as curved lines in order to avoid overlapping with the bonds on the θ lattice.

Let us call such a site a linking site. Thus the one-dimensional lattice may be decomposed into one-dimensional lattices. In two dimensions HC lattice is decomposable into T lattices, and S lattice into S(1, 2) lattices. In three dimensions D lattice is decomposable into FCC lattices, SC lattice into FCC (1, 2) lattices and the BCC into SC(1, 2, 3) lattices. The Bethe lattices are decomposed into cacti or generalized cacti. In Fig. 1 some decomposable lattices and the corresponding sublattices are given. θ is therefore a superposition of I and II. Any cluster of occupied sites on θ is composed of two occupied subclusters on I and II: if two I sites belong to the same cluster on θ , they also necessarily belong to the same cluster on I. The converse is not true: two sites may belong to the same cluster on I, but not necessarily on θ if none of their linking sites on II are occupied. The same holds of course for infinite (percolating, spanning) clusters, which means that percolation occurs in θ only if it occurs simultaneously in both I and II. Hence a rigorous—though trivial—relation is obtained

$$p_c^{\theta} \geq p_c^I = p_c^{II} \tag{1}$$

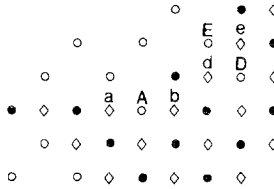


Fig. 2. An example for a cluster on I and the corresponding linking cluster on II. Each sublattice is $S(1,2)$. Solid circles denote occupied sites on I which are part of an infinite cluster; diamond shapes denote linking sites on II. Although a and b are directly connected (as next nearest neighbors) on a normal $S(1,2)$ lattice, they are not on this LC, because A, their linking site on I (denoted by an open circle), is vacant; and the same holds for e and d (nearest neighbors) whose linking sites E and D are also vacant.

Let us try to obtain a more significant result. For this goal we consider a generalized problem: Suppose that I sites and II sites are randomly occupied with different probabilities p_1 and p_2 . What is the condition that the superimposed population percolates on 0? From Eq. (1) we get the necessary trivial condition $p_i \geq p_c^I$ for $i = 1, 2$. It is also obvious that for a fixed p_1 in the interval $[p_c^I, 1]$ there is a critical probability $p_2 = p_c^{II}(p_1)$ which is the threshold probability for percolation on 0. In fact the curve $p_2 = p_c^{II}(p_1)$ is the critical line in (p_1, p_2) plane separating the percolating phase from the nonpercolating one. The probability $p_c^{II}(p_1)$ may be estimated as follows:

Consider the infinite cluster on I (which will be denoted I_{inf}) and all sites on II which link together, on 0, pairs of sites in I_{inf} —call it the linking cluster (LC). The linking cluster is obviously infinite, but not all of its sites are necessarily occupied (unless $p_2 = 1$). Moreover, LC is actually a graph on II, where some of the bonds between normally interacting pairs of sites may be missing—if all the corresponding linking sites on I are vacant and therefore do not belong to I_{inf} (see Fig. 2).

It is clear that if all the sites on LC are occupied ($p_2 = 1$) there is an infinite cluster on 0, which is well above threshold (if $p_1 > p_c^I$). In order to bring the LC, and simultaneously 0 too, down to percolation threshold, II sites should be diluted by exactly $p_c^{II}(p_1)$. If nothing is known of the structure of LC a plausible assumption is that it is similar in some sense to I_{inf} . This may be regarded as a mean field approximation or as an ignorance hypothesis. The dilution factor p_d which brings down I_{inf} to percolation threshold is exactly expressible by p_c^I and p_1 , namely, $p_d = p_c^I/p_1$. With the similarity assumption between LC and I_{inf} we get the obvious estimate:

$$p_c^{II}(p_1) \approx p_c^I/p_1 \tag{2}$$

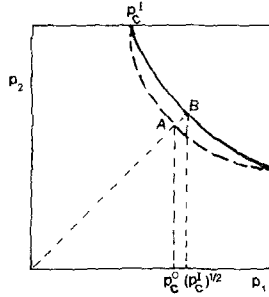


Fig. 3. The critical line in (p_1, p_2) plane for a typical case. The solid line is the approximate hyperbola $p_1 p_2 = p_c^I$. The exact critical line is schematically drawn by a dashed line. It is conjectured that it should always lie below the hyperbola. For a Bethe lattice the hyperbola is indeed the correct result with $p_c^I = 1/(z - 1)^2$. Point A is the exact critical isotropic point at p_c^0 ; B is the approximated one at $(p_c^I)^{1/2}$.

and the critical line in the (p_1, p_2) plane will be

$$p_1 p_2 \approx p_c^I = p_c^{II} \tag{3}$$

which means that it is approximately a hyperbola (see Fig. 3). Let us notice that at least for $p_1 = 1$ or $p_2 = 1$ the relation (3) is trivially exact.

If we are interested only in the “isotropic” case, $p_1 = p_2$, which was the starting point of this discussion, and which is the more conventional percolation problem, we get

$$p_c^0 \approx (p_c^I)^{1/2} \quad \text{or} \quad p_c^I \approx (p_c^0)^2 \tag{4}$$

Let us examine more closely some of the consequences of this estimate, taking advantage of well-known classical exact results.

(i) When 0 is the honeycomb lattice, I is the triangular lattice T: $p_c^I = p_c^T = 0.5$ is exactly known (Sykes and Essam^(1,2)), so that

$$p_c^H \approx (0.5)^{1/2} = 0.707 \tag{5}$$

A good empirical result for p_c^H is 0.6973 ± 0.001 obtained by Vicsek and Kertesz.⁽³⁾

With this result we can be pretty sure that $p_1 p_2 = 0.5$ according to Eq. (3) is indeed a good approximation for the actual critical line. The result of Eq. (5) was recently obtained elsewhere: Joy and Strieder⁽⁴⁾ obtained it, also as an approximation based on effective medium theory of conductivity; Kondor⁽⁵⁾ claims that Eq. (5) should be read as a strict equality. However, this claim is conjecture-dependent, and we believe (see the following discussion) that the correct relation is $p_c^{HC} \leq (0.5)^{1/2}$, i.e., p_c^{HC} is

slightly less than $(0.5)^{1/2}$, which is apparently confirmed by the empirical evidence.

(ii) When 0 is S, the square lattice, I is the S(1, 2) lattice. Here another exact result, due to the matching relation between the two, is known:^(1,2)

$$p_c^s + p_c^{s(1,2)} = 1 \quad (6)$$

Together with relation (4) we get

$$(p_c^s)^2 + p_c^s \approx 1 \quad (7)$$

the solution of which is

$$p_c^s \approx (\sqrt{5} - 1)/2 = 0.618 \quad (8)$$

A good empirical result (Reynolds *et al.*⁽⁶⁾) is $p_c^s = 0.593$. Both results (5) and (8) are in a relatively good agreement with "experiment." The first deviates by about 0.01 and the second by 0.025. Both are overestimates.

(iii) For the one-dimensional lattice Eq. (4) is trivially exact, $p_c^1 = p_c^0 = 1$. Moreover, Eq. (3) is also an exact result for Bethe lattices: If the coordination number of the Bethe lattice is z , then $p_c = 1/(z - 1)$ (Fisher and Sykes⁽⁷⁾). The sublattices here are generalized cacti, the coordination number of which is $z(z - 1)$, but due to the existence of loops its p_c may be easily shown to be $1/(z - 1)^2$, so that $p_c^0 = (p_c^1)^{1/2}$ is a strict equality. This is also true even for the more general lattice where the coordination numbers on 0 of I sites and II sites are not equal.

The detailed results for all systems for which data were available are summarized in Table I. Inspecting Table I, one observes that relation (4) can be invariably replaced by an inequality

$$p_c^0 \leq (p_c^1)^{1/2} \quad (9)$$

where the equality holds only for Bethe lattices (including the one-dimensional case). This result may be interpreted, in fact, as if the linking cluster is not equivalent exactly to I_{inf} but rather it is more abundant or more compact (or both), so that it should be diluted more than I_{inf} in order to reach threshold. It would be expected that relation (3) for the critical line should be replaced by

$$p_1 p_2 \leq p_c^1 \quad (10)$$

Indeed we conjecture that Eqs. (9) and (10) are always correct. Some arguments substantiate the above interpretation and conjecture; let us follow some of them:

(i) The probability \bar{p} that a site on II links at least two occupied sites on I is

$$\bar{p}(p_1) = 1 - np_1(1 - p_1)^{n-1} - (1 - p_1)^n = 1 - np_1q_1^{n-1} - q_1^n \quad (11)$$

Table I. Estimates of p_c^0 for Several Lattices^a

Dimension	Original lattice	Sublattice	P_c^I (empirical)	p_c^0 (empirical)	$(p_c^I)^{1/2}$	$(p_c^0)^{1/2} / P_c^0 - 1 = c$	l
1	linear	linear	1 (exact)	1 (exact)	1	0	1
2	HC	T	0.5 (exact)	0.698	0.707	0.01	1
	S(1)	S(1,2)	0.407	0.593	0.638	0.07	2
3	S(1)	S(1,2)	using matching relation		0.618	0.04	2
	D(1)	FCC(1)	0.198	0.428	0.445	0.04	1
	SC(1)	FCC(1,2)	0.136	0.311	0.369	0.20	2
	BCC(1)	SC(1,2,3)	0.097	0.243	0.311	0.28	4
Bethe lattice	Coordination number z	Generalized cactus	$\frac{1}{(z-1)^2}$ (exact)	$\frac{1}{(z-1)}$ (exact)	$\frac{1}{z-1}$	0	1

^aThe empirical values of the percolation threshold are cited from Stauffer (Ref. 8) when related to simple lattices and from Shante and Kirkpatrick (Ref. 9) when related to lattices with further interaction. l is the maximum possible number of linking sites on Π for a given connected pair on \mathbf{I} .

Table II. Estimates for p_c^0 by Solving $p_1 \bar{p}(p_1) = p_c^1$

Dimension	0	I	p_1	$\bar{p}(p_1)$	$p_c^* = [(p_c^1)^{1/2} + p_1]/2$	p_c^0	$c^* = p_c^*/p_c^0 - 1$
2	HC	T	0.670	0.746	0.689	0.698	-0.013
	S	S(1, 2)	0.543	0.749	0.591	0.593	-0.003
3	D	FCC	0.390	0.507	0.418	0.428	-0.023
	SC	FCC(1, 2)	0.268	0.508	0.318	0.311	0.026
	BCC	SC(1, 2, 3)	0.198	0.491	0.255	0.243	0.048

where n is the coordination number on 0 and $q = 1 - p$. It can be easily shown that

$$\bar{p}(p_1) \geq p_1 \quad \text{for } p_1 \geq 1/(n-1) \quad (12)$$

where the equality holds only for $n = 2$ or $n = 3$ and $p_1 = 1/(n-1)$. We are interested, of course, only in probabilities $p_1 \geq p_c^0 \geq 1/(n-1)$. Hence if the linking sites on II were completely uncorrelated, then the infinite LC would indeed be more abundant than I_{inf} and its dilution factor would be p_c^0/\bar{p} , which is less than p_c^0/p_1 , so that Eqs. (9) and (10) are obtained.

The above consideration led us to a new estimate for p_c^0 as the root of the equation:

$$p_1 \bar{p}(p_1) = p_c^1 \quad (13)$$

The results of this estimate are given in Table II.

The roots of Eq. (13) are invariably smaller than the previous ones, as they should be, but also smaller than the empirical thresholds. Their deviations from the empirical values are mostly of the same order of magnitude as the deviation of $(p_c^1)^{1/2}$. It turns out that (with the exception of the Bethe lattices) the average $[p_1 + (p_c^1)^{1/2}]/2$ may be used as a better estimate for p_c^0 than each of the individual ones. This perhaps indicates that still better results may be obtained by taking into account more and finer details of LC.

(ii) Another argument which makes the conjecture plausible is the following: Consider a new linking cluster, which is the set of all sites on II which are neighbors of at least *one* site on I_{inf} (and not necessarily of two as before). It is trivially true that the pair connectedness function on this linking cluster is at least equal to the corresponding function on I_{inf} . This also indicates (although not rigorously proves) that the dilution factor of II sites should be lower than the dilution factor on I, from which we obtain again our conjectures (9)–(10).

(iii) A further indication is an "empirical" one. By construction randomly large (but finite) clusters in I (with $p_1 \sim p_c^0$) and studying the structure of the corresponding linking clusters it is always obtained that the

linking cluster is more abundant, and also more compact—the average number of its bonds per site is greater than the number for the primary cluster on I. This has been checked for square and honeycomb lattices.

(iv) The last indication to the validity of the conjecture is the fact that the relation (9) is a strict equality for Bethe lattices, which are in a sense a limiting case of actual lattices. It may be expected that for them the ratio $(p_c^l)^{1/2}/p_c^0$ gets its minimum, 1. It seems that all these are plausible arguments, but they still do not furnish a solid proof to the conjecture.

Coming back to the results of Table I we notice that although all of them obey the inequality (9), their deviation from equality, measured by the index $c = (p_c^l)^{1/2}/p_c^0 - 1$, vary. For Bethe lattices $c = 0$, for HC and D it is fairly small, for the other lattices it is much bigger. This effect is indeed reasonable: The assumption of similarity between LC and I_{inf} which led to Eq. (4) is plausible where for each pair of directly interacting occupied sites on I there is just one linking site on II. This is true for HC, D, and Bethe lattices, whereas for all other lattices, l , the maximum number of linking sites, is 2 or 4 [e.g., for the square lattice, the pair (0, 0) and (1, 1) is directly connected on I and has two linking sites (0, 1), and (1, 0); for BCC the pair (0, 0, 0) and (1, 0, 0) on I has four linking sites: $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, and $(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$]. It is expected therefore that the linking cluster is relatively more abundant the higher is l , and hence p_c^0 should be relatively smaller. Indeed for both dimensionality 2 and 3, the index c increases with l .

However, it is clear that l itself is not the only factor that determines c , e.g., Bethe lattice with $z = 4$, HC, and D all have the same l and still differ by c . It is reasonable to believe that both dimensionality and length of minimal loop in each lattice also play a significant role in determining the critical probability.

3. CORRELATED PERCOLATION

The above considerations are applicable also to some correlated problems. As an illustration we apply them to the “polychromatic” correlated site problem. This problem may be relevant to the understanding of the properties of supercooled water as proposed by Stanley.⁽¹⁰⁾ The formulation of this specific problem is the following: In a square (or diamond) lattice each site is linked by four bonds to other sites. Let the bonds be randomly occupied with probability p . Sites which are surrounded by four occupied bonds are called “green.” The problem is to find the critical probability for percolation of the green sites.

Evidently p^g , the occupation probability of the green sites, is

$$p^g = p^4 \quad (14)$$

but the green sites are correlated (e.g., if it is known that a certain site is green, the probability of any of its nearest neighbors being green is $p^3 > p^4 = p^g$). However, decomposing the original lattice into two sublattices [each S(1,2) or FCC(1)], the green sites on each are totally uncorrelated (Gonzales⁽¹¹⁾), because no two sites on I have a bond in common. Still, the exact formulation of this problem as a site percolation problem is quite complicated for the following reason: Once the population of the green site is randomly established on I, the green sites on II are correlated both with the I sites and among themselves. However, naive considerations, similar to the ones already used for the uncorrelated problem, would lead again to an estimate for the percolation threshold p_c^g :

The green sites percolate on I, hence

$$p_c^g \geq p_c^I \quad (15)$$

Owing to the positive correlation on 0 it is intuitively expected that

$$p_c^g < p_c^0 \quad (16)$$

The green sites have also to percolate on the linking cluster on I. Each linking site has already at least two occupied bonds (with which it is linked to two green sites on I_{inf}). Hence, the probability that it is also green is at least $p^2 = (p^g)^{1/2}$. Repeating the previous arguments for the present problem we get

$$p_c^I \approx p_c^g (p_c^g)^{1/2} = (p_c^g)^{3/2} \quad (17)$$

or

$$p_c^g = (p_c^I)^{2/3} \quad (17a)$$

The numerical results are, by using the known empirical p_c^I values,

$$\begin{aligned} \text{for square lattice } (p_c^g)^S &= 0.550 \\ \text{for diamond lattice } (p_c^g)^D &= 0.34 \end{aligned} \quad (18)$$

The corresponding empirical results obtained by Monte Carlo calculation are $(p_c^g)^S = 0.562$ (Blumberg *et al.*⁽¹²⁾), and—preliminary result— $(p_c^g)^D = 0.35$ (Blumberg and Stanley⁽¹³⁾). In fact the latter empirical result was obtained for the ice lattice, but presumably the result for the diamond is very close to it. Both estimates deviate by about 0.01 from the empirical values, which may be regarded as very good approximations. Let it be stressed, however, that unlike the estimates for the uncorrelated problem, the present ones are higher than the empirical values and the reason is quite clear: When I_{inf} is given, the occupation probability of the linking cluster is also given. If correlation among green sites on II is neglected, the probability p_ν of a II site to be green, provided it has exactly ν green neighbors on I,

is

$$p_\nu = \left[p \left(\frac{1 - p^3}{1 - p^4} \right) \right]^{4-\nu}, \quad \nu = 2, 3, 4 \tag{19}$$

the relative weight for this event is

$$W_\nu = \binom{4}{\nu} p^{4\nu} (1 - p^4)^{4-\nu} \tag{19a}$$

Thus we get the probability that a site on the linking cluster is green (Shlifer⁽¹⁴⁾)

$$p_{\nu \geq 2} = \frac{\sum_{\nu=2}^4 W_\nu p_\nu}{\sum_{\nu=2}^4 W_\nu} = p^2 \frac{6 - 8p^3 + 3p^6}{6 - 8p^4 + 3p^8} \tag{20}$$

This expression is less than p^2 as assumed before. The neglect of this effect influences the estimate for p_c^g to be too low. Substituting $(p_c^g)^{1/2}$ in Eq. (16) by $p_{\nu \geq 2}$ of Eq. (20) and solving it, we get new estimates 0.61 for $(p_c^g)^S$ and 0.38 for $(p_c^g)^D$. Both results are now too high because the effects of the structure of LC, discussed in the previous section, were ignored. It is hoped that by taking all the important effects into consideration the correct values will be more closely reproduced. However, it is very remarkable that when both structure and correlation effects are neglected the estimates are so close to the empirical values.

Similar “green” problems may be defined for other lattices. If we define on the honeycomb lattice a green site as a site with three occupied bonds, the estimate for threshold is given by

$$(p_c^g)^{HC} \approx (p_c^1)^{3/4} = (0.5)^{3/4} = 0.595 \tag{21}$$

This value has not yet been empirically calculated and it is given here as a prediction.

4. CONCLUSION

By very elementary arguments about the structure of the infinite cluster in the site percolation problem, a few approximate relations have been obtained among p_c of decomposable lattices and the p_c of the corresponding sublattices. By heuristic arguments we could establish these relations as inequalities, which are conjectured to be always true. This method, although not universal, is still applicable to some of the most commonly used lattices. It is also very satisfying that it may be extended to correlated percolation, and also to a generalized two-parameter “anisotropic” site problem, for which critical lines are obtainable in an approximate way.

No attempt has been made here to produce critical exponents or relations among them. A priori it seems that the present method will fail to achieve this goal, because at least one of the sublattices (and in the isotropic problem both) are way off the critical region, as $p_c^0 - p_c^1$ is usually not a very small number.

Nor did we try to get the exact shape of the critical line in the anisotropic problem (except for the Bethe lattice). In our simplest estimate we got it as a hyperbola, but a more detailed examination of the problem may reveal some finer features. There are some indications that the critical line in a real lattice is perpendicular to the lines $p_1 = 1$ and $p_2 = 1$, or at least form less acute angles than the first approximation yields. This behavior will be studied in the future. Some other problems will be treated in the future: We will try to establish a more rigorous proof for the central conjecture [Eqs. (9) and (10)]. Also an attempt will be made to find more accurate relations among threshold probabilities, in order to improve the estimates and replace the approximate and the inequality signs by an equality sign, even though it would probably involve infinite series. It is hoped, however, that the first few terms of the series will be more easily calculated than by other methods.

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