

Convergence of Mean-Field Approximations in Site Percolation and Application of CAM to $d=1$ Further-Neighbors Percolation Problem

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We study the mean-field approximation in the site-percolation problem. Using the analog of the Simon–Lieb inequality, we show that the mean-field critical probability is convergent to the exact value when the size of clusters tends to infinity. Applying this approximation to the one-dimensional further-neighbor percolation problem and calculating some critical coefficients, we prove that the asymptotic scaling relations predicted by the coherent-anomaly method are satisfied.

KEY WORDS: Site-percolation problem; mean-field approximation; critical probability; critical exponents.

1. INTRODUCTION

One-dimensional models very often can be solved exactly and hence provide us with a very good test of approximate methods such as the renormalization group approach, Monte Carlo simulations, etc. This also concerns one-dimensional percolation models, for which exact results have been found for an arbitrary range of bonds n (holes of width up to $n-1$ do not separate an animal).^(1,2) It was shown in these papers that the critical probability p_c^* is equal to unity for any n , but some critical exponents are n -dependent. Namely: $\beta=0$ (the percolation probability in the vicinity of p_c^*), $\gamma=n$ (the mean cluster size), $\nu=n$ (the correlation length), $\eta=1$ (the correlation length at p_c^*), $\delta=\infty$ (the reaction of the percolation probability on “ghost field”), $\alpha=2-n$ (specific heat); in the

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parentheses, we have put the quantities whose behavior is described by the corresponding exponents. The simplicity of this model and its rich critical behavior have inclined us to use it as a test of the general scheme to study phase transitions which was introduced by one of us (M.S.), namely the coherent-anomaly method (CAM).^(3,4)

The general idea of the CAM when applied to magnetic models can be sketched as follows: First, let us recall that in the Weiss mean-field approximation, an infinite system of interacting spins is replaced by a system of noninteracting spins merged into some effective field h^{eff} . This field is subsequently determined from the consistency condition, which for translationally invariant systems states that h^{eff} is proportional to the magnetization of the system. This crude method can, however, be improved. We can assume that the interacting system is replaced by a non-interacting finite clusters of spins merged into h^{eff} . All interactions inside clusters are treated exactly and h^{eff} is again determined from a similar consistency condition. Such an approximation is called a cluster mean-field approximation. When the size of the clusters tends to infinity, we expect that the solutions obtained by the cluster mean-field approximation are convergent toward the exact solution and that the corresponding critical coefficients show the so-called coherent anomaly. For example, the critical coefficient $\bar{\chi}$ describing the mean-field-like divergence of the susceptibility

$$\chi \sim \bar{\chi} \varepsilon^{-1}, \quad \varepsilon = \frac{T - T_c}{T_c} \quad (1.1)$$

has the form

$$\bar{\chi} \sim \Delta^{-\gamma+1}, \quad \Delta = \frac{T_c - T_c^*}{T_c^*} \quad (1.2)$$

for large clusters. The symbols T_c and T_c^* stand for the mean-field and the exact critical temperatures, respectively. Hereafter we usually omit the term ‘‘cluster’’ when referring to the cluster mean-field approximation. Relations similar to (1.2) can also be written for other quantities and allow us to determine T_c^* and critical exponents very accurately.

Although the CAM relations are numerically well confirmed⁽⁵⁾ even for the percolation problem,⁽⁶⁻⁸⁾ their derivation is based on some scaling assumptions and more rigorous results concerning this scheme would be very desirable. Until now, such results have been obtained only for the one-dimensional Ising model, the spherical model, and the Gaussian model.⁽⁹⁾

In the present paper we calculate the mean-field critical probability p_c and some critical coefficients for the above-mentioned one-dimensional per-

colation model with arbitrary range of bonds n . Our results confirm that the relations predicted by the CAM are satisfied for the investigated model.

In Section 2 we introduce the concept of a local “ghost field” which allows us to write the condition for determining p_c in a simple and general form. Using this condition and the analog of the Simon–Lieb inequality^(10,11) proved for the percolation problem by Aizenman and Newman,⁽¹²⁾ we show that as the size of clusters tends to infinity, the obtained series of p_c is convergent toward the exact value. This result is very general and also can be applied to any d -dimensional model. In Section 3 we calculate p_c explicitly for the considered model and show that our result converges to the exact value in accordance with the finite-size scaling.⁽¹³⁾ The calculation of some critical coefficients is presented in Section 4, where we also prove that asymptotically relations predicted by the CAM are satisfied. Section 5 contains a summary of our results.

2. MEAN-FIELD APPROXIMATION AND ITS CONVERGENCE

In the mean-field approximation for Ising models the critical temperature is determined from the condition⁽⁹⁾

$$1 = \beta \sum_{b \in \partial L} \langle S_0 S_b \rangle_L \quad (2.1)$$

where $\beta = 1/k_B T$ and summation of the two-spin center-to-border correlation functions is performed over boundary sites of the cluster L . This equation follows from the expansion of the self-consistency condition around the critical point. The aim of this section is to obtain a similar condition in the site percolation problem and to investigate some of its consequences.

To start with the site percolation problem, let us recall the definition of the generating function for the number of animals of size s (per site):

$$G(h) = \sum_{s=1}^{\infty} p_s (1-h)^s \quad (2.2)$$

where p_s is the probability that the central site 0 belongs to an animal of the size s . In order to derive the analog of (2.1) we have to replace a uniform “ghost field” h by a local “ghost field” h_k . This leads to the following generating function $G(\{h_k\})$:

$$G(\{h_k\}) = \sum p^s q^r (1-h_{k_1})(1-h_{k_2}) \cdots (1-h_{k_{s-1}}) \quad (2.3)$$

where p denotes the probability that a given site is occupied, $q = 1 - p$, and r stands for the size of the perimeter.⁽¹⁴⁾ The summation is performed over

all lattice animals which are connected to the site 0. The factor $(1 - h_k)$ appears provided that the site k belongs to a given animal. It is obvious that if we put all h_k equal to each other, then we obtain the expression (2.2). Our generalization enables us, however, to write the pair correlation function C_{0k} in a very simple form:

$$C_{0k} = \frac{-\partial G(\{h_i\})}{\partial h_k} \quad (2.4)$$

The derivative in (2.4) is calculated in the limit $h_j \rightarrow 0$ for $j = 1, 2, \dots$. The validity of (2.4) follows from the fact that nonzero contributions to C_{0k} come only from those terms of $G(\{h_i\})$ for which the site k is occupied. Summation of these terms yields C_{0k} , because the correlation function is equal, from the definition, to the probability that sites 0 and k are occupied and connected by any animal.

To obtain the mean-field approximation in the site percolation problem, let us suppose that the central site belongs to a certain cluster L (other mean-field approaches to the site percolation problem can be found in refs. 7, 8, and 15). To avoid confusion, we would like to emphasize that a cluster is a certain set of sites on the lattice. On the other hand, what we here refer to as an animal is a given configuration of occupied and connected sites. As is well known, the role of a "ghost field" reduces to that of a factor diminishing the probability p_s . This is a consequence of the fact that the field connects a given animal to the infinite (or percolating) animal. Such an interpretation suggests the possibility of introducing the mean-field approximation by the following modification of $G(\{h_i\})$:

$$G(\{h_k\}) = \sum p^s q^r (1 - h_{k_1})(1 - h_{k_2}) \cdots (1 - h_{k_{s-1}})(1 - P')^m \quad (2.5)$$

where P' is the probability that a boundary site of the cluster L is connected to the infinite animal (by homogeneity, the probability is the same for each boundary site, but this can be easily generalized to the case with nonequivalent boundary sites), and m is the number of boundary sites in the given animal (i.e., m stands for the number of sites placed on the boundary of the cluster L). The summation in (2.5) is performed over all animals which can occupy the given cluster L .

There is a simple formula which enables us to write the percolation probability P that the site 0 is connected to the infinite animal, using the generating function G .⁽¹⁴⁾ With the use of this formula and (2.3) we can write

$$P = \sum p^s q^r [1 - (1 - h_{k_1})(1 - h_{k_2}) \cdots (1 - h_{k_{s-1}})(1 - P')^m] \quad (2.6)$$

where $0 \leq h_k \leq 1$. The summation in (2.6) is performed over all animals which are included in the given cluster L and which connect the site 0 to the border of the cluster. The self-consistency condition

$$P' = P \tag{2.7}$$

leads to the equation

$$P = \sum p^s q^r [1 - (1 - h_{k_1})(1 - h_{k_2}) \cdots (1 - h_{k_{s-1}})(1 - P)^m] \tag{2.8}$$

The critical probability p_c defined as the probability at which a nonzero solution of (2.8) vanishes (for $h_k = 0$) can be found as the solution of the following equation:

$$1 = \frac{\partial}{\partial P} [\text{rhs of (2.8)}] \tag{2.9}$$

where derivative is calculated for $P \rightarrow 0$ and for $h_k \rightarrow 0$ ($k = 1, 2, \dots$). It is easy to show that in this limit we have

$$\frac{\partial}{\partial P} = \sum_{k \in \partial L} \frac{\partial}{\partial h_k} \tag{2.10}$$

Hence, Eq. (2.9) can be equivalently written in the form

$$1 = \sum_{b \in \partial L} C_{0b}^L \tag{2.11}$$

Here C_{0b}^L is the center-to-border correlation function calculated for all animals which are included in the given cluster L and which connect the site 0 to the border of the cluster.

With the use of the Simon–Lieb inequality,^(10,11) it has been shown⁽⁹⁾ that for the Ising model, the mean-field critical temperature calculated as a solution of (2.1) is convergent in the limit of infinite cluster size to the exact value. The condition (2.11) suggests that a similar proof should also exist in the percolation problem. To show that this is really the case, we use the analog of the Simon–Lieb inequality proved for the percolation problem by Aizenman and Newman.⁽¹²⁾ The essence of our method is, however, very similar to that presented in ref. 9.

The Aizenman–Newman inequality can be written now as follows:

$$C_{0k} \leq \sum_{b \in \partial L} C_{0b}^L C_{bk} \tag{2.12}$$

Here the summation is performed over all the sites which belong to the border ∂L . If we want to tackle the further-neighbor percolation problem,

then our definition of C_{0k} and C_{0k}^L has to allow some “holes” in the path. As the proof does not depend on such details, the inequality (2.12) is satisfied also in this general case.

To prove the convergence

$$\lim_{R \rightarrow \infty} p_c = p_c^* \quad (2.13)$$

for the cluster size R , let us suppose that $p < p_c$ for certain L . Then

$$\sum_{b \in \partial L} C_{0b}^L = C_0 < 1 \quad (2.14)$$

The inequality comes from the fact that C_{0b}^L is an increasing function of the probability p . By iterating (2.12) l times, where $l = [k/R]$, we obtain

$$C_{0k} \leq C \exp(-m_0 R[k/R]) \quad (2.15)$$

where $m_0 = -R^{-1} \ln C_0$, and C is some constant value. The exponential decay of the correlation function (2.15) implies $p < p_c^*$. Now let us suppose that $p < p_c^*$. This implies an exponential decay of the correlation function C_{0k} . Thus, for large L , we obtain

$$\sum_{b \in \partial L} C_{0b}^L < \sum_{b \in \partial L} C_{0b} \xrightarrow{R \rightarrow \infty} 0 < 1 \quad (2.16)$$

We can then deduce that $p < p_c$. This, together with the previous conclusion, proves (2.13). We should emphasize here that this proof implies that p_c always approaches p_c^* from below.

3. CALCULATION OF p_c

To determine the critical probability p_c explicitly in the one-dimensional model, let us suppose that our cluster is a chain consisting of $2R + 1$ sites. Before solving this problem in a general case, we find solutions in some simple cases.

3.1. Case $n = 1$

This case corresponds to the usual percolation problem where even a single hole disconnects an animal. The correlation function C_{0R}^L is equal to

$$C_{0R}^L = p^R \quad (3.1)$$

According to (2.11), the critical probability can be found as the solution of the following equation:

$$1 = 2p_c^R \quad (3.2)$$

Asymptotically for $R \gg 1$, the solution of (3.2) can be written in the form

$$q_c = 1 - p_c \sim \frac{\ln 2}{R} \quad (3.3)$$

Of course, in the limit $R \rightarrow \infty$, our solution is convergent to the exact value $p_c^* = 1$.

3.2. Case $n = 2$

In this case, to calculate the correlation function C_{0R}^L , we have to include all animals with single holes. If our animal consists of k holes, then $R - k$ sites must be occupied and there are

$$\binom{R-k}{k}$$

ways of distributing holes between the occupied sites. Thus,

$$C_{0R}^L = \sum_{k=0}^{R'} \binom{R-k}{k} p^{R-k} q^k = p^R \sum_{k=0}^{R'} \binom{R-k}{k} a^k = p^R a_R \quad (3.4)$$

where $a = q/p$, $R' = \max\{k: R - k \geq k\}$,

$$a_R = \sum_{k=0}^{R'} \binom{R-k}{k} a^k$$

To sum this series, let us notice that a_R is the R th term in the expansion

$$f(x) = \sum_{R=0}^{\infty} a_R x^R \quad (3.5)$$

where

$$f(x) = \frac{1}{1 - x - ax^2} \quad (3.6)$$

Hence, $a_R = f^{(R)}(0)/R!$ and further calculations are rather straightforward. We write the function $f(x)$ in the form

$$f(x) = \frac{A}{x - x_1} + \frac{B}{x - x_2} \quad (3.7)$$

where A, B are constants and x_1, x_2 are roots of the denominator in (3.6). Differentiation of (3.7) yields

$$a_R = \frac{A}{x_1^R} + \frac{B}{x_2^R} \quad (3.8)$$

For large R , the term with the smallest root (x_1) is dominant:

$$a_R \rightarrow \frac{A}{x_1^R} \quad (3.9)$$

Using both (2.11) and the explicit form of A and x_1 , we can find the critical probability p_c as the solution of the following equation:

$$1 = 2C_{0R}^L = \frac{2}{(1 + 4a_c)^{1/2}} \left(\frac{q_c}{(1 + 4a_c)^{1/2} - 1} \right)^R \quad (3.10)$$

where $a_c = q_c/p_c$. For large R , a_c is small and our solution has the asymptotic form

$$q_c^2 \sim \frac{\ln 2}{R} \quad (3.11)$$

It should be pointed out here that this result is quite similar to (3.3).

3.3. General Case

In the general case our method of calculation of C_{0R}^L is very similar to that for the case $n = 2$. We have to take into account all configurations with k_1 single holes, k_2 double holes, ..., k_{n-1} $(n-1)$ -holes, subject to the condition that

$$R - N \geq k_1 + k_2 + \dots + k_{n-1} \quad (3.12)$$

where

$$N = k_1 + 2k_2 + \dots + (n-1)k_{n-1} \quad (3.13)$$

Thus we can write

$$C_{0R}^L = p^R a_R \quad (3.14)$$

where

$$a_R = \sum \binom{R-N}{k_1} \binom{R-N-k_1}{k_2} \dots \times \binom{R-N-k_1-k_2-\dots-k_{n-2}}{k_{n-1}} a^N \quad (3.15)$$

Fortunately, a_R can also be found as the R th term in the expansion (3.5), but the function $f(x)$ is given now by

$$f(x) = \frac{1}{1 - x - ax^2 - a^2x^3 - \dots - a^{n-1}x^n} \quad (3.16)$$

We skip the rather elementary analysis and say only that the function (3.16) can be expressed in a form similar to (3.7). Analogously, for $R \gg 1$ only the smallest root (x_1) gives dominant contributions to a_R . Although an analytic expression for this root for arbitrary n is unavailable, it is enough to get its asymptotic (in the limit $a \rightarrow 0$) expansion. After some calculation we obtain

$$x_1 = \begin{cases} 1 - a + a^2 - \dots + a^n - 2a^{n+1} + O(a^{n+2}) & n \text{ even} \\ 1 - a + a^2 - \dots - a^n + O(a^{n+2}) & n \text{ odd} \end{cases} \quad (3.17)$$

Substitution of (3.17) into (3.9) leads to an expression which can be written in the form

$$q_c^n \sim \frac{\ln 2}{R} \quad (3.18)$$

for small a and arbitrary n . Of course, (3.18) encompasses the cases $n = 1$ and $n = 2$. We emphasize here that the result (3.18) implies that

$$q_c \sim R^{-1/n} = R^{-1/\nu} \quad (3.19)$$

since we have $\nu = n$ in our model.⁽²⁾ Equation (3.19) shows that the difference between the exact critical probability $q_c^* = 0$ and the approximate ones q_c calculated by the mean-field approximation and by the finite-size scaling⁽¹³⁾ scales in the same way.

4. CRITICAL EXPONENTS β AND ν

To calculate the exponent β , which describes the behavior of the percolation probability P near p_c^* ,

$$P \sim (\varepsilon^*)^\beta \quad (4.1)$$

where $\varepsilon^* = (p - p_c^*)/p_c^*$, we have to find the critical coefficient \bar{P} which describes mean-field behavior of P near p_c :

$$P \sim \bar{P} \varepsilon^{\beta_0} \quad (4.2)$$

where β_0 is the mean-field exponent and $\varepsilon = (p - p_c)/p_c$. The coefficients \bar{P} and β_0 can be easily found by expanding (2.8) around p_c for small P (for details, see ref. 7). Finally, we obtain

$$\beta_0 = 1 \quad (4.3)$$

and

$$\bar{P} = \frac{p_c F'(p_c)}{G(p_c)} \quad (4.4)$$

where

$$F(p_c) = \sum m p_c^s q_c^r \quad (4.5)$$

and

$$G(p_c) = \frac{1}{2} \sum m(m-1) p_c^s q_c^r \quad (4.6)$$

In (4.5) we can separately sum the series with $m=1$ (an animal connected to the border by one site) and with $m=2$ (by two sites). In the first case, we have to sum up all the correlation functions C_{0N}^L , where $R \leq N \leq 2R$, and in the second case, we have to find C_{02R+1}^L . Because m can only be equal to 0, 1, or 2, in (4.6) we have to sum up all animals only with $m=2$. This corresponds to calculating the correlation function C_{02R+1}^L . Then

$$F(p_c) = 2q_c^n \sum_{N=R}^{2R} C_{0N}^L + 2C_{02R+1}^L \quad (4.7)$$

and

$$G(p_c) = C_{02R+1}^L \quad (4.8)$$

Direct summation in (4.7) and (4.8) can be done in an analogous way as in Section 3. Thus we present here only the final result:

$$F(p_c) = 2[1 - (1 - p_c)^n]^R \quad (4.9)$$

and

$$G(p_c) = [1 - (1 - p_c)^n]^{2R} = \frac{1}{4} \quad (4.10)$$

The last equality in (4.10) follows from the fact that the equality $F(p_c) = 1$ determines the critical probability p_c [this condition is equivalent to

(2.11)]. Substituting (4.9) and (4.10) into (4.4) and using (3.19), it is easy to obtain the asymptotic formula:

$$\bar{P} \sim R^{1/n} \tag{4.11}$$

But from (3.19), the asymptotic behavior of \bar{P} can be equivalently written as

$$\bar{P} \sim q_c^{-1} \tag{4.12}$$

and the critical exponent β is equal to

$$\beta = \beta_0 - 1 = 0 \tag{4.13}$$

for any n , in agreement with exact calculations.⁽²⁾

To calculate the exponent γ , which describes the divergence of the mean cluster size S near p_c^* ,

$$S \sim (\varepsilon^*)^{-\gamma} \tag{4.14}$$

we have to find the critical coefficients \bar{S} which describe the mean-field-like divergence of S in the vicinity of p_c^* :

$$S \sim \bar{S} \varepsilon^{\gamma_0} \tag{4.15}$$

The mean cluster size S can be calculated in the following way^(7,14):

$$S = \frac{\partial P}{\partial h} \tag{4.16}$$

To find (4.16), we have to put $h_k = h$ in (2.8) for $k = 1, 2, \dots$. Then differentiation yields

$$S = \frac{H(p_c)}{1 - F(p_c)} \tag{4.17}$$

where

$$H(p_c) = \sum s p_c^s q_c^r \tag{4.18}$$

and the summation is performed over all animals which are included in the given cluster L . The resulting series have a structure similar to that of the derivative of geometrical series and can be easily evaluated using the technique described in Section 3. The final analytic formula is rather lengthy, and we write here only an asymptotic estimation of (4.18) as

$$H(p_c) \sim R^{2-1/n} \tag{4.19}$$

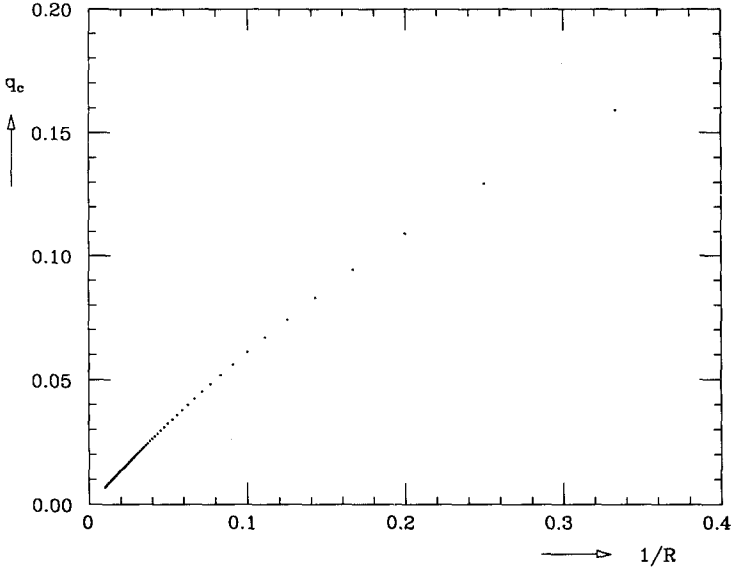


Fig. 1. The parameter q_c as a function of $1/R$ for $n=1$.

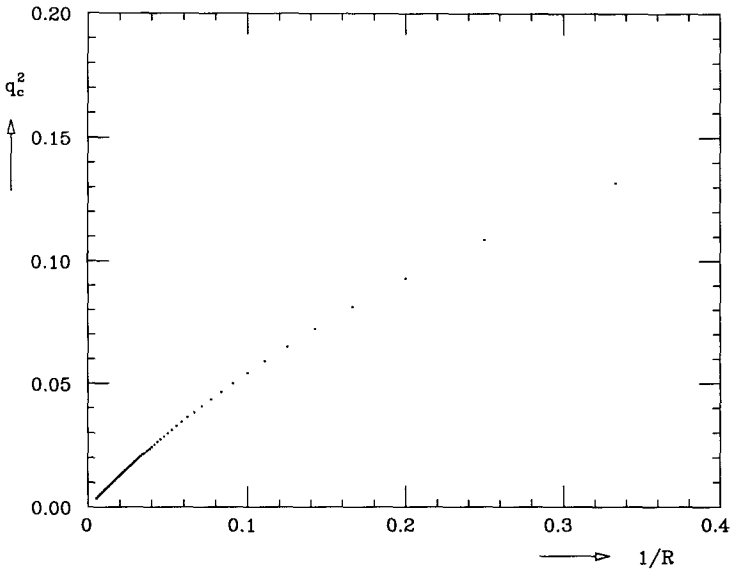


Fig. 2. The quantity q_c^2 as a function of $1/R$ for $n=2$.

Using (4.15), (4.19), (4.9), and (4.17), we can write

$$\bar{S} = \frac{H(p_c)}{p_c F'(p_c)} \sim R^{1-1/n} \tag{4.20}$$

Then relation (3.19) allows us to write

$$\bar{S} \sim q_c^{-n+1} \tag{4.21}$$

This leads to the following value of the exponent γ :

$$\gamma = n - 1 + 1 = n \tag{4.22}$$

in agreement with ref. 2.

To make our analysis more transparent, we present some results obtained by numerical calculations. We choose chains with $3 \leq R \leq 100$ as clusters. All quantities were calculated directly by summing up the corresponding combinatorial series without any asymptotic estimations. Figures 1 and 2 present plots of q_c^n as a function of $1/R$ for $n=1$ and 2, respectively. The evident linearity in the limit $1/R \rightarrow 0$ confirms the relation (3.19). Figures 3 and 4 present the inverse of the critical coefficient \bar{P} as a function of q_c for $n=1$ and 2, respectively. In Fig. 5 we plot \bar{S} as a function of q_c for $n=1$. In the limit $q_c \rightarrow 0$, \bar{S} apparently approaches some finite

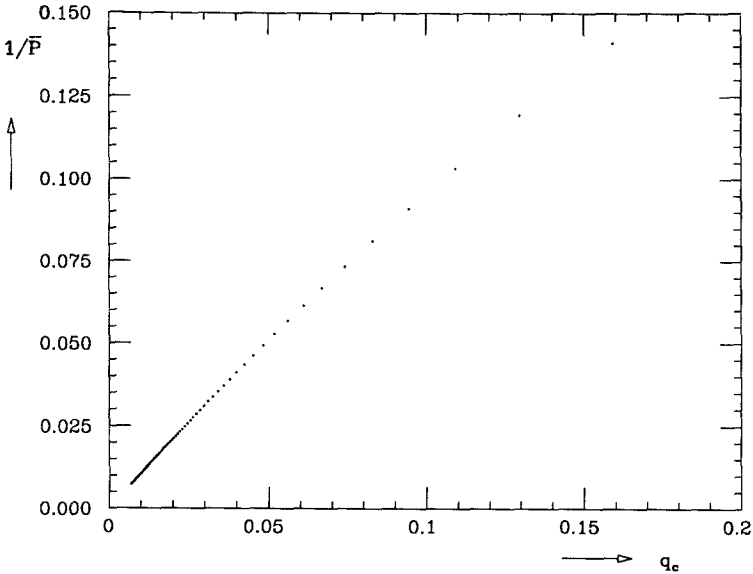


Fig. 3. The inverse of the percolation probability coefficient as a function of q_c for $n=1$.

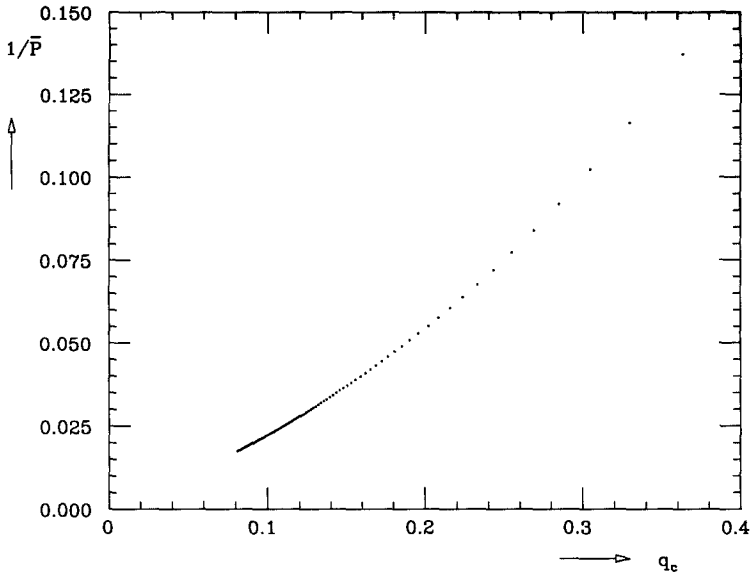


Fig. 4. The inverse of the percolation probability coefficient as a function of q_c for $n=2$.

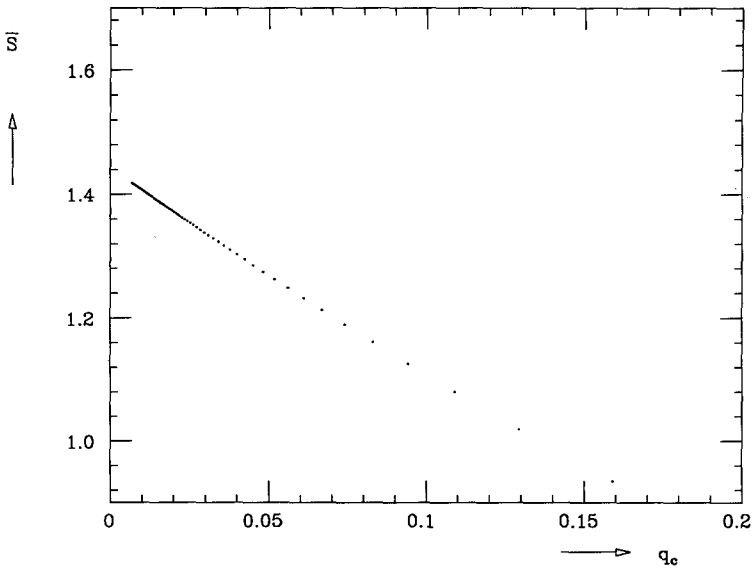


Fig. 5. The mean cluster size coefficient \bar{S} as a function of q_c for $n=1$.

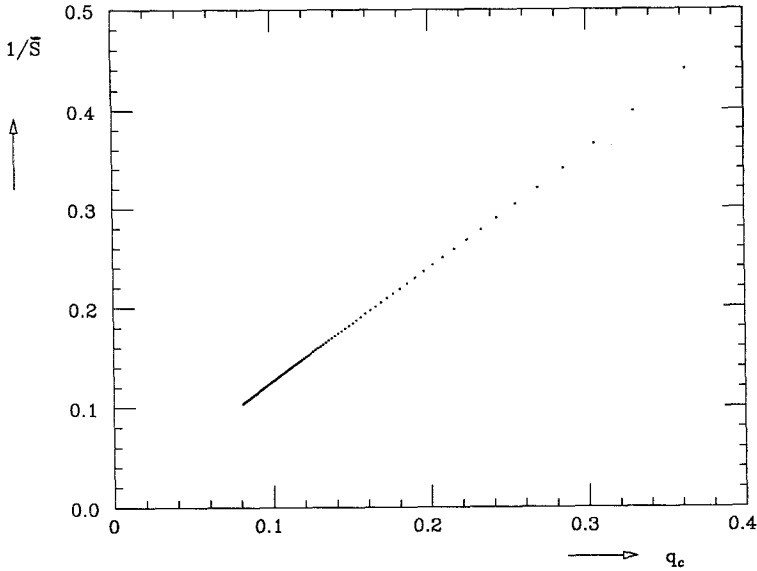


Fig. 6. The inverse of the mean cluster size coefficient \bar{S} as a function of q_c for $n=2$.

value. Thus we can conclude that $\bar{S} \sim q_c^0$ (constant), in agreement with (4.21). The analogous plot for $n=2$ is presented in Fig. 6. Comparing the figures corresponding to $n=1$ and $n=2$, we can conclude that the convergence of the results in the latter case is much slower. We can explain this feature by investigating the next to the leading term Δ in the asymptotic expansion (3.18), namely

$$q_c^n \sim \frac{\ln 2}{R} (1 + \Delta) \quad \text{where} \quad \Delta \sim R^{-\Delta_1} \tag{4.23}$$

By numerical estimations, we have found that for $n=1$ and 2, $\Delta_1 = 1$ and 0.6, respectively. For higher values of n , the exponent Δ_1 has a smaller value. This implies a slower convergence of the obtained results.

5. CONCLUSIONS

In the first part of this paper, we investigated some general properties of the mean-field approximation for the site-percolation problem. Introducing the concept of local “ghost fields,” we showed that the mean-field critical probability can be found as a solution of the equation which has a very close counterpart in magnetic systems. Using the analog of the Simon–Lieb inequality for correlation functions, we proved that the mean-

field critical probability is smaller than the exact value for finite clusters and that it converges to the exact value in the limit of infinite cluster size. In the second part of this paper, we applied the mean-field approximation to the one-dimensional further-neighbor percolation problem. Calculations of the critical probability and some critical coefficients enabled us to confirm, in the limit of infinite cluster size, certain relations predicted by the coherent-anomaly method (CAM). We believe that relations predicted by the CAM for other exponents are also rigorously satisfied in this limit.

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NOTE ADDED IN PROOF

After submitting our paper we realized that another proof of (2.13) was given by X. Hu in his Ph.D. Thesis.

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