Approximations of mean spherical type for lattice percolation models

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Abstract. We develop a general class of approximations of mean-spherical (MSA) type as a method for studying lattice percolation problems. We review the MSA and test certain extensions of it on lattice spin models. The relations between thermal spin models and percolation models are then reviewed in order to identify natural extensions of the MSA to percolation models. These extensions are used to treat both site and bond percolation models. In one 'low-density' formulation of MSA, the threshold for bond percolation on a lattice is found to equal the value at the origin of the corresponding lattice Green's function. This formula gives accurate results for all lattices studied, and in all space dimensions $d \geq 3$. An accurate treatment is also given of the general site-bond problem. The entire percolation locus for this problem agrees closely with the results of simulation. We also introduce a new method for studying percolation transitions which is a hybrid of the Kikuchi cluster approximation scheme and the MSA. The method is shown to give good values for percolation thresholds while preserving the valuable features of the standard MSA. In particular, it provides a convenient means of computing the pair connectedness function. We also explore extensions of our approximations to treat directed site and bond percolation.

1. Introduction

Percolation is a phenomenon defined by the formation of macroscopic clusters in a many-body system, given a criterion for pairwise connectedness†. It has been studied in recent years from at least two different points of view. Those studying percolation as a particularly accessible, geometrical analogue of a phase transition seek an accurate method to locate the percolation threshold and to study the scaling behaviour of physical quantities in its vicinity. On the other hand, those who want to study the influence of percolation on bulk material properties and transport processes in disordered materials and liquids want an account of various key quantities that describe clustering, such as the average coordination number of a particle and the mean cluster size, throughout the entire range of system parameters. For example, the influence of ionic clustering upon the specific conductance of electrolytes is a subject of current interest in physical chemistry [1].

The solution of integral equations for the connectedness function (and its relatives) has been shown to yield a detailed, powerful approach to the latter class of problems. Several such integral equations have been derived and solved, both for continuum and

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† We make the standard distinction between connectivity and connectedness: the former describes the (constant) properties of the graph or lattice on which a percolation process is defined; the latter describes the properties of clusters generated by that process; see e.g. [2].

lattice percolation [2-8, 13]. The challenge of consistently incorporating into this approach information about the percolation locus has received much less attention. This paper is a contribution toward that effort.

One such integral equation approximation which has been studied for various continuum percolation models is the Ornstein–Zernike equation with closure provided by the mean spherical approximation (MSA). This approximation was originally developed [9] for nearest-neighbour thermal spin models and their equivalent lattice-gas analogues. It was subsequently generalized [10] to longer-range lattice models and to continuum fluid models. The MSA for a continuum system of particles at thermal equilibrium can be defined by the equations

$$h(x_{12}) = -1 \qquad x_{12} \leqslant a$$
$$c(x_{12}) = -\beta v(x_{12}) \qquad x_{12} > a. \tag{1.1}$$

Here, $h(x_{12})$ and $c(x_{12})$ are, respectively, the full correlation function and the direct correlation function between particles at the vector positions x_1 and x_2. Here, $x_{12} = |x_1 - x_2|$ is the scalar distance between such particles, $v(x_{12})$ is their pairwise potential energy, and $\beta = (kT)^{-1}$, where T is the absolute temperature and k is Boltzmann's constant. The distance a is the distance of closest approach fixed by a hard-core potential which is part of the pairwise interaction. The MSA has been used profitably [11, 12] to treat a wide variety of thermal problems. A major benefit of this approximation is that the resulting equations, e.g. for the equation of state, can be solved analytically for many models of interest.

In 1983, the MSA was extended [3] to the random-sphere percolation model, to give a relation between the two-point connectedness function $g_c(x)$ and the direct connectedness function $c_c(x)$ of that model. This is a model of randomly placed spheres which are taken to be directly connected if their pairwise separation is less than a fixed distance a, the sphere diameter. For this model, the MSA is equivalent to the Percus–Yevick approximation for percolation, which was first suggested by Coniglio *et al* [2] in work that extended the cluster-expansion treatment of $g_c(x)$ by Hill [23]. More general models have been introduced by considering systems of particles in thermal equilibrium interacting via a pair potential $\phi(x)$, which introduces correlation between the centres of particles (if one sets $\phi(x) = 0$ the model reduces to the random-sphere percolation model). A number of such continuum systems of interest can be solved exactly in the MSA [3-5]. It is also natural to apply the MSA to the functions $g_c(x)$ and $c_c(x)$ in lattice percolation models. A recent study of MSA for lattice site percolation by Høye and Stell [6] found that both the percolation threshold and critical exponents for percolation on certain lattices in three and higher dimensions are predicted accurately. In this paper, we extend that study by using certain general methods of MSA type to investigate lattice bond and site-bond percolation. The critical exponents are found to be the same as in site percolation, as one expects, while the bond percolation threshold is predicted accurately on all lattices studied, and in all dimensions $d \geqslant 3$. In this paper, we will work with a very general class of approximations of MSA type. These approximations, in general, define a closure of the Ornstein–Zernike equation by providing a pair of assumptions corresponding to the two given in (1.1). In general:

(i) The volume surrounding each lattice site is divided in two by choosing a sphere that surrounds that site. The value of the pair correlation function (either $h(x)$ or $c(x)$ can be used), giving the interaction of a site with other sites inside the chosen sphere, is provided explicitly, either by the constraints of the model itself, or by some other

approximation. Many approximation schemes provide such values for correlation functions at small separation.

(ii) The interaction with lattice sites outside the sphere is described by giving an approximate form, for large separation, of the direct correlation function $c(x)$. In the original MSA, as given by (1.1), the radius of the sphere in the scheme just described is taken to be the exclusion radius, defined as the range of the hard-core part of the potential, and the closure is specified at small separation by giving the values of $h(x)$ inside the exclusion sphere. We note that the scheme just outlined has obvious similarities with the effective medium approximation (EMA) [14, 15]. It also has basic differences; for example, it gives, in general, critical exponents that are non-classical. For random percolation, the MSA yields critical exponents $\gamma = 2$, $\eta = 0$, in three dimensions, compared with the results $\gamma = 1.80$, $\eta = -0.07$ given by series estimates. These results were developed in detail for site percolation in [6]; they apply without change to the models discussed here.

Our results for percolation thresholds are all reasonable estimates; some of them agree with estimates from series analysis and transfer-matrix methods to three decimal places. nevertheless, we do not consider our method to be a serious competitor to these specialized methods for locating critical points, at least in its present state of evolution. Our emphasis lies rather in providing a global description of percolation models: we offer a method for calculating connectedness functions that agree with low-density series approximations, give reasonably good descriptions of the entire percolation locus, and show reasonable, albeit not exact, critical exponents.

This paper is organized as follows. In section 2 we review the general procedure for solving the MSA for thermal lattice models. We illustrate the use of MSA-like approximations by applying these to the Ising model. In section 3 we discuss the relation between thermal models and percolation models in order to identify natural extensions of the MSA framework to percolation. We review the earlier treatment of site percolation. Appropriate variants of the MSA are then applied to both bond and site-bond percolation. In section 4 we discuss the use of the Kikuchi cluster approximation to obtain the short-distance values of $h(x)$ needed to complete an MSA-like closure. In section 5 we apply MSA-like approximations to directed site and bond percolation models. Section 6 discusses the present limitations of the approximations discussed in this paper, and gives suggestions for further research. Section 7 summarizes our conclusions.

2. General MSA formalism

In this section we review the general Ornstein–Zernike formalism for thermal lattice models. We illustrate its use by applying it to the nearest-neighbour Ising model, as described in lattice-gas terminology. Our emphasis is on identifying general strategies for creating approximations of MSA type.

The Ornstein–Zernike equation is

$$h(x_{12}) = c(x_{12}) + \rho \sum_{x_3} c(x_{13}) h(x_{32}). \tag{2.1}$$

In this section we use the terminology of thermal physics, in which $h(x_{12})$ and $c(x_{12})$ are, respectively, the full pair correlation function and direct pair correlation function. The sum in (2.1) is over all lattice sites. We note that the function $h(x)$ and other

functions defined on a lattice depend upon a vector which we denote as x or x_{ij}; this is the separation of sites i and j. An equation identical to (2.1) governs the relation between the pair connectedness function $g_c(x)$ and direct connectedness function $c_c(x)$, in a percolation model. The appropriate subsidiary conditions, which must be used with this equation to give a closed computational scheme, are, however, different in thermal models and in percolation models. This will be discussed in detail in the next section.

We indicate the Fourier transform of a function, e.g. $c(x)$, by placing a caret over the corresponding function symbol. Thus we have

$$c(x) = \frac{\Omega}{(2\pi)^3} \int \hat{c}(k) \, e^{-ik\cdot x} \, d^3k. \tag{2.2}$$

Here the integral over the wavenumber k is over a single Brillouin zone of the lattice. Also, Ω is the volume of the Wigner–Seitz cell associated to a single lattice site; it is here normalized to unity. Taking the Fourier transform of both sides of (2.1) allows an algebraic solution for $\hat{h}(k)$ in terms of $\hat{c}(k)$:

$$\hat{h}(k) = \frac{\hat{c}(k)}{1 - \rho\hat{c}(k)}. \tag{2.3}$$

The strategy for solving (2.1) is this: since $c(x)$ is assumed to be short-ranged, $\hat{c}(k)$ can be written explicitly in terms of a small number of unknown constants, namely the different values of $c(x)$ which are non-negligible. Substituting an assumed form for $\hat{c}(k)$ in (2.3) and Fourier-transforming then gives a solution for $h(x)$. Boundary conditions and constraint conditions specify the remaining constants in the solution. These conditions contain the physical assumptions specific to the model being studied.

Specifically, for the problems of interest in this section, we assume that $c(x_{12})$ is non-zero only if x_{12} is either zero or equal to a nearest-neighbour lattice vector, in which cases $c(x)$ takes the values c_0 and c_1, respectively. Substituting this information in the transform inverse to (2.2) then gives, for hypercubic lattices,

$$\hat{c}(k) = c_0 + 2c_1 \sum_{i=1}^{d} \cos k_i a. \tag{2.4}$$

Here a is the lattice spacing and d is the dimensionality of the lattice. For the sake of algebraic simplicity, we specialize our discussion to hypercubic lattices and will work, unless otherwise stated, with the three-dimensional simple cubic (SC) lattice. The discussion of this paper applies, however, to general Bravais lattices.

Taking the Fourier transform of (2.3) and adding to both sides the identity

$$\delta_{x,0} = \frac{\Omega}{(2\pi)^3} \int \frac{1 - \rho\hat{c}(k)}{1 - \rho\hat{c}(k)} \, e^{-ik\cdot x} \, d^3k \tag{2.5}$$

then gives

$$\delta_{x,0} + \rho h(x) = \frac{\Omega}{(2\pi)^3} \int \frac{1}{1 - \rho\hat{c}(k)} \, e^{-ik\cdot x} \, d^3k. \tag{2.6}$$

Using (2.4) for $\hat{c}(k)$ allows us to rewrite the denominator of the RHS as

$$1 - \rho\hat{c}(k) = z\rho c_1\left((1 + K^2) - d^{-1} \sum_{i=1}^{d} \cos k_i a\right). \tag{2.7}$$

Here z is the coordination number for the lattice, and the quantity K^2 is given by the expression

$$K^2 \equiv z\kappa^2 \equiv \frac{1 - \rho c_0 - z\rho c_1}{\rho c_1}. \qquad (2.8)$$

Substituting (2.7) into (2.6) gives

$$\delta_{x,0} + \rho h(x) = \frac{1}{z\rho c_1} \frac{\Omega}{(2\pi)^3} \int \frac{e^{-ik \cdot x}}{(1 + \kappa^2) - d^{-1} \Sigma_{i=1}^{d} \cos k_i a} \, d^3k$$

$$\equiv \frac{zG(x)}{z\rho c_1}. \qquad (2.9)$$

This last equation defines $G(x)$, which can be identified as the Green function of the lattice version of the Helmholtz wave equation with wavenumber $K^2 = z\kappa^2$. This function occurs frequently in mathematical physics and has been tabulated [16, 17]. We note in particular that for $\kappa^2 = 0$, the function $zG(x)$ is the generating function for random walks on the lattice being studied.

We digress briefly to justify our identification of κ, as defined by (2.8), with the inverse correlation length. For convenience, define $\chi(x) \equiv \delta_{x,0} + \rho h(x)$. Then we have

$$\frac{\hat{\chi}(0)}{\hat{\chi}(k)} = \frac{1 + \rho\hat{h}(0)}{1 + \rho\hat{h}(k)} = \frac{1 - \rho\hat{c}(k)}{1 - \rho\hat{c}(0)} \qquad (2.10)$$

where the second step uses the Ornstein–Zernike equation (2.3). Expanding the RHS of (2.10) in powers of k^2 and substituting (2.4) gives

$$1 + \Lambda_2(ka)^2 + O[(ka)^4] \qquad (2.11)$$

with k^2 the norm squared of the vector k and Λ_2 defined by

$$\Lambda^2 = \frac{\rho c_1}{1 - \rho\hat{c}(0)}. \qquad (2.12)$$

For simple hypercubic lattices, Λ_2 can equivalently be identified as [18, 19]

$$\Lambda_2 = \frac{\Sigma_x x^2 \chi(x)}{\Sigma_x \chi(x)}. \qquad (2.13)$$

That is, Λ_2 is the second spherical moment of the quantity $\chi(x)$ divided by its zeroth moment. To see this, write $\chi(x)$ in terms of its Fourier transform, replace the factors of x with k-derivatives, and note that (2.11) is a Taylor series. Direct comparison then shows that $z\Lambda_2 = \kappa^{-2}$, with κ^2 defined by (2.8). The singular part of the susceptibility near a critical point is proportional to the volume integral of $h(x)$, i.e. to $\hat{h}(0)$. According to (2.3), we can then identify such a point by the condition

$$\rho\hat{c}(0) = 1. \qquad (2.14)$$

Note that by (2.8), this is equivalent to the condition $\kappa^2 = 0$. Also, it is reasonable to identify Λ_2 with the square of the correlation length and thus identify $\kappa^{-2} = \xi^2$. The correlation length defined in this manner has the same critical behaviour as that based on the assumption that $h(x)$ decays exponentially; the former definition is, however, more generally applicable. For example, even when $h(x)$ has algebraic decay, as it will when $c(x)$ does, this definition is still applicable, providing that the second moment of $c(x)$ exists [11].

Several further relations are useful for the general discussion of critical behaviour as described by the Ornstein–Zernike equation. To develop these, we write G_0 and G_1, respectively, for the values of the Green function $G(x)$, defined by (2.9), evaluated for a lattice displacement vector equal, respectively, to zero, and to the vector difference between a pair of nearest neighbours. We can specify these displacement vectors as $x = 0$, and $|x| = a$, respectively. Note that this causes no ambiguity because, by symmetry, $G(x)$ takes the same value for all nearest-neighbour displacement vectors. In the special case that $\kappa^2 = 0$, which defines the critical point, we write these same quantities as $\bar{G}_0$ and $\bar{G}_1$, respectively. Similarly, the values of $h(x)$ at $x = 0$ and $|x| = a$ are written h_0 and h_1, respectively. Setting $|x| = a$ in (2.9) then gives

$$\frac{zG_1}{z\rho c_1} = \rho h_1. \tag{2.15}$$

Dividing (2.9) for $x = |a|$ by the same equation, with $x = 0$, gives

$$\frac{zG_1}{zG_0} = \frac{\rho h_1}{1 + \rho h_0}. \tag{2.16}$$

Finally, we can relate G_0 and G_1, for a SC lattice, by using the identity

$$\frac{\Omega}{(2\pi)^3} \int \frac{d^{-1} \Sigma_{i=1}^d \cos k_i a}{(1 + \kappa^2) - d^{-1} \Sigma_{i=1}^d \cos k_i a} \, e^{-ik \cdot x} \, d^3 k = zG_1. \tag{2.17}$$

(A similar identity holds for any lattice.) This follows directly by using the symmetry of a Bravais lattice and the definition of G_1. This gives directly, using (2.5) and (2.9),

$$(1 + \kappa^2) zG_0 - zG_1 = 1. \tag{2.18}$$

This relation can be used to eliminate G_1 from (2.16) and give a basic relation for the critical point:

$$\frac{z\bar{G}_0 - 1}{z\bar{G}_0} = \frac{\rho h_1}{1 + \rho h_0}. \tag{2.19}$$

We note that the lattice-gas density ρ occurs explicitly only in the combinations ρc_0, ρc_1. Two further constraints must now be supplied to completely specify an MSA-like closure of the Ornstein–Zernike equation. In standard applications of the MSA to pair correlation functions, these are chosen to be the vanishing of the correlation $h(x)$ inside the interaction hard core, and the equation $c(x) = -\beta v(x)$ outside this core. Here $v(x)$ is the interparticle potential and $\beta = 1/kT$. The second of these equations is a 'linear-response' high-temperature approximation; it is exact to first order in β and the potential $v(x)$. For the Ising model, this implies $h_0 = -1$ and $c_1 = K$ where $K = -\beta J_{LG}$ and J_{LG} is the lattice-gas coupling constant, related to the Ising model coupling constant J_{Ising} by

$$J_{LG} = 4 J_{Ising}. \tag{2.20}$$

Substituting these relations into (2.15) and (2.19) then gives the condition for criticality:

$$\rho(1 - \rho) K_{crit} = \bar{G}_0. \tag{2.21}$$

Because we consider the high-temperature, zero-field Ising model only, we have, for the lattice-gas density, $\rho = 0.5$. Thus

$$K_{crit} = 4\bar{G}_0 \sim 1.08 \tag{2.22}$$

for the three-dimensional SC lattice. This should be compared with the value $K_{crit} = 0.840$ given by the second Bethe-Peirls approximation for this lattice, and also with the value $K_{crit} = 0.918$ given by high-temperature series analysis [20], which represents the most precise means available for estimating such quantities.

We derive a variant of this approximation if we recall the definition of $c(x)$ as the direct correlation function and write the density-independent (but temperature-dependent) approximation

$$c(x) = f(x) = e^{-K} - 1. \tag{2.23}$$

This approximation is exact to first order in the lattice-gas density, i.e. it is the first term in the Mayer expansion. Using c_1 from (2.23) gives the criticality condition

$$K_{crit} = -\ln(1 + 4\bar{G}_0) \tag{2.24}$$

which implies $K_{crit} = 0.732$. Thus for the SC Ising model in three dimensions, the estimates for the critical point given by the high-temperature approximation (2.22) and the low-density approximation (2.24) are of comparable accuracy. It is (2.22) (or in general the constraint $c(x) = -\beta v(x)$) that has come to be called the MSA (because (2.22) proves to be exact in the mean-spherical and spherical models of a magnetic system). As we shall see, in some percolation problems, in which $h(x)$ is replaced by the pair connectedness function and $c(x)$ by the direct connectedness function, it turns out that (2.23) (or in general $c(x) = \exp(-\beta v(x)) - 1$) appears to be the more natural and generally useful approximation. This is also found to be the case in studies of continuum percolation [5].

3. The MSA for site and bond percolation

In this section, we will apply the Ornstein-Zernike formalism of section 2 to lattice percolation models. First, the case of site percolation is reviewed. We then show that a natural extension of the MSA to bond percolation gives an analytic formula for the critical density that was previously proposed on empirical grounds by Sahimi and co-workers [21] as an accurate, general approximation for this quantity. Finally, we give an approximation of MSA type for the general case of random site-bond percolation and reproduce the complete percolation locus for that model.

The formalism of section 2 can be directly applied to percolation models because these satisfy an Ornstein-Zernike equation of the form (2.1). In particular, one has [2]

$$g_c(x_{12}) = c_c(x_{12}) + \rho \sum_{x_3} c_c(x_{13}) g_c(x_{32}) \tag{3.1}$$

with $g_c(x_{12})$ and $c_c(x_{12})$, respectively, being the connectedness function and direct connectedness function, respectively. The Ornstein-Zernike equation can be taken to be a definition of $c(x)$, and thus has no content *per se*. However, we focus here on the 'derivation' of this equation from other representations, in particular those based on Mayer series; these will suggest good approximations for the value of $c_c(x)$ and $g_c(x)$ for small separation. This is necessary because one requires an independent second relation between $c_c(x)$ and $g_c(x)$ in order to have a closed set of equations for these quantities. Below, we shall refer to both the ρ and β expansions of $c_c(x)$ and $g_c(x)$, which facilitate estimation of $c_c(x)$ for small argument. In the case of random or uncorrelated percolation, g_c and c_c are temperature-independent, so that only the

ρ-expansion is available. We focus in particular on mappings of percolation models onto limiting cases of thermal models; these allow us to draw on our experience with MSA-like approximations for the latter. Such mappings allow us to exploit the machinery of liquid-state physics. Also, they are essential when thermal correlations are imposed between the sites or bonds of a percolation model.

One can calculate virial series for $c_c(x)$ and $g_c(x)$ using graph-theoretic formalism. In the absence of thermal correlations, an elegant way to do this is via a formulation due to Essam [22] in terms of self-avoiding walks. An equivalent, computationally powerful, formalism [24] for calculating $d(G)$ involves the Mayer graphs of the s-state Potts model in the $s \to 1$ limit. For example, for pure site percolation one has

$$g_c(x) = \sum_G d(G)\rho^{v(G)} \tag{3.2}$$

where the sum is over one-irreducible, two-rooted subgraphs G of the lattice being studied, $v(G)$ is the number of vertices in the graph G and $d(G)$ is a purely combinatoric quantity depending only on the graph G. The function $c_c(x)$ is given by a similar expression, but with the sum restricted to non-nodal graphs [22, 24].

To develop series expansions for $g_c(x)$ and $c_c(x)$ in the presence of thermal correlations, it is natural to follow Hill [23] and Coniglio *et al* [2]. Specifically, we write the Boltzmann factor for a thermal model as a sum of two terms:

$$\exp(-v(x_{12}))$$
$$= [\exp(-\beta v(x_{12}))p_b(x_{12})] + [\exp(-\beta v(x_{12}))(1 - p_b(x_{12}))]$$
$$= e^+(x_{12}) + e^*(x_{12}). \tag{3.3}$$

This induces a corresponding separation of the Mayer function

$$f(x_{12}) = f^+(x_{12}) + f^*(x_{12}) \tag{3.4}$$

with $f^+ = e^+$ and $f^* = e^* - 1$. The function $p_b(x_{12})$ defines the separation-dependent probability of a bond between two particles. Its choice is dictated by the physical phenomenon to be modelled. The first term in (3.3) is identified with the particles being directly connected, the second with them *not* being directly connected. Substitute the sum (3.4) for each Mayer bond in the virial expansions of $h(x_{12})$ and $c(x_{12})$, and expand each Mayer graph into subgraphs whose lines correspond to f^+- or f^*-bonds. Define [2, 24] the connectedness function $g_c(x_{12})$ to be the sum of all such subgraphs in the expansion of $h(x)$ in which the root points are joined by a chain of f^+-bonds; the blocking function $g_b(x_{12})$ is the sum of all the remaining subgraphs. Similarly, define the direct connectedness function $c_c(x)$ to be the sum of the corresponding subgraphs contributing to $c(x)$; this is equivalent to the set of subgraphs contributing to $g_c(x)$ that *in addition* have no nodal points. These definitions are compatible with (3.1). Thus the correlation function has been written as the sum

$$h(x_{12}) = g_c(x_{12}) + g_b(x_{12}) \tag{3.5}$$

of the two-point connectedness function and two-point blocking function. One can show [24] that $g_c(x_{12})$ as defined above formally is in fact the two-point connectedness function for a many-body system of particles having correlation function $h(x)$ and density ρ, and being pairwise-connected with separation-dependent probability $p_b(x)$. The connectedness function $g_c(x_{12})$ is the probability distribution associated with finding particles at x_1 and x_2 in the same connected cluster. Similarly, $g_b(x_{12})$, the

two-point blocking function, is the corresponding probability distribution associated with the particles at x_1 and x_2 being in *different* clusters. We note that our probability-density definition of $g_c(x)$ and the corresponding definition of $c_c(x)$ induced by (3.1) are not dependent on the density series expansions of these quantities; the latter are not fully general. One expects such series to represent $g_c(x)$ and $c_c(x)$ only for ρ and β that characterize non-percolating states; as yet only partial results are available [7, 25] for their radii of convergence. We note that, in general, one cannot give a separate physical interpretation in terms of probability densities, of $c_c(x)$, because, unlike $g_c(x)$, it need not be positive definite.

It has been shown [8] that the expansion procedure of Hill can be carried out elegantly by using the isomorphism [25] between percolation and the one-state limit of the s-state Potts model. Specifically, the one-state limit of a continuum Potts model [8] with interparticle potential

$$V_{ij} = \phi(x_{ij}) + v(x_{ij})(1 - \delta_{\sigma_i \sigma_j}) \tag{3.6}$$

gives a correlated continuum percolation model with interparticle potential $\phi(x)$ and separation-dependent bond probability $p_b(x)$. If one develops Mayer expansions for the thermodynamic quantities of the model defined by (3.6), and applies the operator $\mathrm{d}/\mathrm{d}s|_{s=1}$ to them, they yield the basic quantities in the description of the corresponding percolation model. This procedure provides a realization of the general percolation process described below (3.5), with each pair of particles connected with a separation-dependent bond probability given by

$$p_b(x) = 1 - \exp(-\beta v(x)) \tag{3.7}$$

with $v(x)$ as in (3.6). If we write the Ornstein–Zernike equation (2.1) for the specific case of the s-state Potts model, take the $s \to 1$ limit and, use identities [8, 24]

$$h(x_1, \alpha, x_2, \beta) \to -g_c(x_{12}) \tag{3.8}$$

$$c(x_1, \alpha, x_2, \beta) \to -c_c(x_{12}) \tag{3.9}$$

we recover (3.1). Here α and β are any two different spin states.

When we restrict the continuum Potts model to a lattice, by imposing the added restriction that particles only occupy positions whose coordinates are integers, the result is a Potts lattice gas [26] whose one-state limit is a very general percolation model. Before doing this, we add to the potential $\phi(x_{ij})$ in (3.6) a delta-function potential interaction that prevents overlap of two lattice-gas particles, and thus of two sites in the resulting percolation model. We then set the function $p_b(x)$ equal to p_b, a nearest-neighbour bond probability for $|x| = a$, and equal to zero for $x \neq a$. The lattice site and bond percolation models are given by special cases $p_b = 1$ and $\rho = 1$, respectively.

The simplest percolation models can also be related to thermal lattice models in other ways. For example, pure bond percolation is the $s \to 1$ limit of the s-state lattice Potts model. Site percolation is the one-state limit of a Potts model containing multisite interactions [27]. It can also be realized as the zero-temperature limit of a site-dilute Ising model [28]. The latter correspondence has been used by Kikuchi [29] to calculate values of the connectedness functions at small separation. In this and the following sections of this paper, we use these mappings to construct MSA-like approximations for specific percolation models. We will use the same terminology as in section 2, but by h_0, h_1 we will mean $g_c(x)$ evaluated at $x = 0$ and $|x| = a$, respectively. Similarly, by c_0, c_1 we denote $c_c(x)$ for $x = 0$ and $|x| = a$, respectively. The random, nearest-neighbour

site-percolation model has already been studied using the MSA [6] approach. In this case it is natural to choose

$$h_0 = 0 \qquad h_1 = 1 \tag{3.10}$$

the former because we must forbid multiple occupation of sites, as just discussed, and the latter because neighbouring occupied sites are always connected. Substituting (3.10) into (2.19) gives the critical site density for percolation

$$\rho_{crit} = \frac{z\bar{G}_0 - 1}{z\bar{G}_0}. \tag{3.11}$$

This is found numerically to be a good approximation in general [6].

For hypercubic lattices, the MSA just described gives p_c to high accuracy for $d \geq 4$. However, in three dimensions, the scheme gives $p_c = 0.341$, where series analysis gives 0.312 ± 0.003 [30]. This discrepancy suggests that an optimal MSA for site percolation has yet to be found. We note that the EMA [14] for the conductivity of a site-disordered resistor lattice has similar difficulties. The EMA is very similar in spirit to the hybrid approximations to be discussed next. Although this scheme gives excellent approximations in two dimensions, it also predicts [15] a three-dimensional site percolation threshold which is too low by 10%.

As already discussed, continuum percolation has many similarities to site percolation as well as bond percolation. Thus the difficulty just discussed may also account for the need to add correction terms [5] to the naive MSA for random continuum percolation in order to recover a good estimate of the critical point in this model. These matters are under investigation.

In the case of bond percolation, we keep the first equation of (3.10), but must modify the second. One possibility is to follow the intuitive notion that the direct connectedness function $c(x_{12})$ should be the probability density associated with having a direct bond between the sites at x_1 and x_2:

$$c_1 = p_b. \tag{3.12}$$

Using the Potts model correspondence, and keeping only terms to first order in ρ, also gives this approximation. Thus this form of the MSA is guaranteed to be appropriate in conditions of low bond density; in terms of the related Potts model, p_b is also a 'high-temperature' expansion variable (see (3.7)). Also, we set $\rho = 1$ because all sites are occupied in bond percolation. This gives for the bond percolation threshold

$$(p_b)_{crit} = \bar{G}_0. \tag{3.13}$$

Sahimi *et al* [21] noted from numerical comparison that this relation provided an extremely good approximation for all regular lattices, and in all dimensions $d \geq 3$. It is very satisfying that an intuitively reasonable form of the MSA gives just this result. Table 1 shows the quality of the estimate (3.13) for a variety of three-dimensional lattices, as well as hypercubic lattices in higher dimensions.

We could have instead made the high-temperature approximation

$$c_1 = K \tag{3.14}$$

where K is defined by the correspondence between the Potts model coupling constant, and the bond probability in the percolation model which is its one-state limit:

$$p_b = 1 - e^{-K}. \tag{3.15}$$

This gives the critical condition

$$(p_b)_{crit} = 1 - \exp(-\bar{G}_0) \sim 0.223. \tag{3.16}$$

Table 1. Approximations to the bond percolation threshold given by (3.18).

Lattice	Series expansions	Monte Carlo	$\bar{G}_0$
Simple cubic	0.2488 ± 0.0002†	0.2493 ± 0.0002‡	0.252 73
Body-centred cubic	$0.180\,25 \pm 0.000\,15$†	—	0.174 15
Face-centred cubic	0.119 ± 0.001†	0.125 ± 0.005§	0.112 06
Hexagonal close-packed	—	0.124 ± 0.005§	0.112 06
Four-dimensional simple cubic	$0.160\,05 \pm 0.000\,15$†	0.1435 ± 0.001†	0.156
Five-dimensional simple cubic	$0.118\,19 \pm 0.000\,04$†	0.118 ± 0.001†	0.115

This table was adapted from [21] and revised.
Sources: †[36], ‡[39], §[40].

This should be compared with (3.13), which gives a value of 0.252, and the existing series analysis results, which give 0.2488 ± 0.0002. Thus (3.16) is a reasonable approximation, but it lacks the remarkable accuracy of (3.13). A similar result is found [5] in studies of continuum percolation, where a form for $c(x)$ must be assumed over the entire range of values for which $v(x)$ is non-zero. In that case also, the low-density ansatz (3.12) is found to give a prediction for the threshold which is numerically superior to the high-temperature ansatz (3.14).

We make the observation that approximations for the short-range values of $c(x)$ would be better motivated if in fact that quantity were a probability density; in fact, it seems never to be positive-definite. This can be easily checked for the problems studied here because $c(x)$ takes only two values, c_0 and c_1. For both pure site and pure bond percolation, it is always found that for any lattice studied that $\rho c_1 > 0$ and $\rho c_0 < 0$. If this were not true, then critical percolation, in the MSA, would be directly isomorphic to a random-walk model [31] defined by transition probabilities ρc_0, ρc_1. However, since having a non-zero value for c_0 simply rescales the time coordinate describing the progress of a random walk, one can always rescale the other non-zero values of c_i by $(1 - \rho c_0)$ and get a physically realizable random walk. In fact, we can rewrite the basic equation (2.15) in a way that is applicable to MSA-like approximations in which $c(x)$ is not assumed to vanish for $x > 1$:

$$\frac{zG_1}{(1 - \rho c_0)} = \rho h_1. \tag{3.17}$$

The existence of this formal equivalence between critical percolation and random-walk models is seen to be a general fact about all MSAs, even those for anisotropic or directed percolation models, as we discuss in section 5. However, in general, the coefficients c_i oscillate in sign, thus higher-order approximations do not give realizable walks. We note that the normalization condition for the transition rates in such a random walk is just the criticality condition for the model being studied (e.g. see (2.14)).

Since the MSA gives a good approximation to the threshold for both pure site and pure bond percolation, it is natural to use it to study the general site–bond percolation model, in which a cluster is defined to be a group of occupied sites connected by occupied bonds. As before, there are several natural approximations that one can use to close the Ornstein–Zernike equation. Note that (3.11) is, *a priori*, just as reasonable an assumption in the general site–bond problem as in the pure bond problem. Using it in the general problem, however, gives a percolation locus in the (ρ, p_b) plane defined by

$$\rho p_b = \bar{G}_0 \tag{3.18}$$

which, e.g. in the case of pure site percolation, is immediately seen to be a very poor approximation.

Thus, we find it more profitable to approximate h_1 by enumerating the smallest graphs that contribute to it, i.e. the smallest bond sets that join two sites that are nearest neighbours. This is equivalent to using the Potts lattice-gas mapping described below (3.8) and calculating the Mayer expansion of that model. On the SC lattice, considering just the two graphs of figure 1 gives

$$h_1(\rho, p_b) = p_b + (1 - p_b) * [1 - (1 - \rho^2 p_b^3)^4] \sim p_b + (1 - p_b) 4 \rho^2 p_b^3. \qquad (3.19)$$

This approximation for h_1 is exact for site percolation, and gives, for bond percolation, the critical value $(p_b)_{crit} = 0.258$, whereas the approximation based on (3.12) gives 0.252 for the same quantity. The best series estimate gives $p_b = 0.2488$. The percolation locus in the (ρ, p_b) plane as given by the approximation (3.16) is shown in figure 2. This locus has been obtained by simulation in both two dimensions [32] and three dimensions [33]. The critical locus given by substituting (3.19) in (2.19) is found by calculating the critical site density ρ, for a specific value of p_b, by using the Newton–Raphson method. This approximation is already of high quality and can easily be improved by
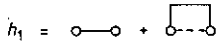
Figure 1. The lowest-order graphs in the density expansion of h_1, the nearest-neighbour connectedness function, as given by (3.19). This quantity is required in the MSA for a general site–bond percolation model. Full and broken lines represent p_b and $(1 - p_b)$ respectively.
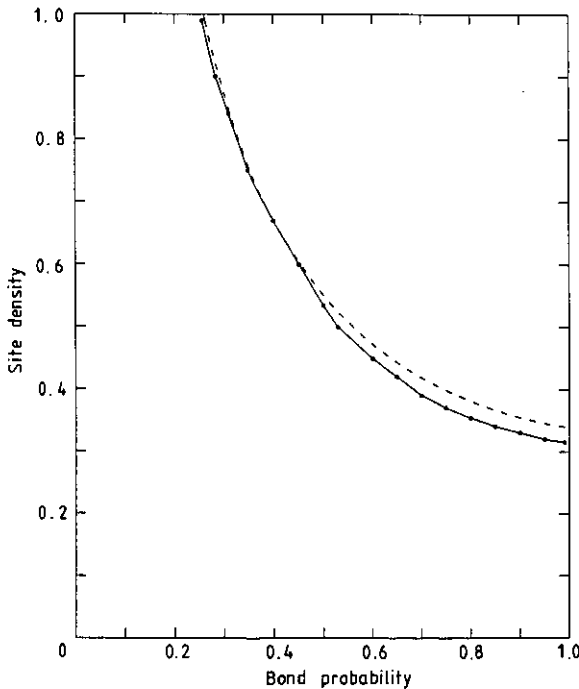
Figure 2. The percolation locus for random site–bond percolation on the three-dimensional SC lattice, as given both by simulation (full line), and by the MSA of section 3 (broken line).

adding terms, except for the part of the phase plane near the pure site percolation limit; we discuss this problem further in section 5. It is worth noting that many different schemes are available for estimating the quantity h_1 in both thermal and percolation models. In particular, the method of Kikuchi [34, 35] involves assuming a functional form for the free energy which contains as parameters the values of $h(x)$ for small separation x, and minimizing this functional to determine these quantities. We discuss this class of approximations in the next section.

4. Hybrids of the Kikuchi cluster approximation and MSA

In section 3, we showed that one can obtain good estimates for phase transition loci from MSA-like approximation schemes if reasonable estimates are available for values of the correlation functions at short range. In this section, we explore the possibility of using the Kikuchi cluster variational method (CVM) [34, 35] to determine these. In order to complement our discussion in section 3 of the basis of an MSA approach to percolation models, we also obtain directly a Kikuchi CVM for bond percolation, by using the Fortuin–Kastelyn mapping [25] between percolation and the Potts model. We compare the direct estimates of the critical bond probability given by this method with hybrid estimates given by using the structural information from this method as input to MSA-like approximations. The hybrid estimates are found to be superior. The CVM, first systematically developed by Kikuchi [34, 35], involves several steps. We outline these here, restricting our discussion to the Ising-like spin models for which the theory was originally developed:

(i) Because Ising variables take discrete values, the various small clusters of contiguous spins (pairs, triplets, etc.) can take on only a finite number of possible configurations. After specifying a set of small clusters to serve as a basis set, one chooses as working variables the probabilities of occurrence of each possible configuration of these clusters. If the basis set consists of only one cluster, a nearest-neighbour pair, the corresponding occurrence probabilities are just the values of the spin-spin correlation function at nearest-neighbour separation. We note that these variables are exactly the quantitites needed in the MSA-like approximations discussed in this paper. Direct use of these values yields the well-known Bethe approximation.

(ii) In terms of the working variables, one writes a consistent approximation for the free energy of the system. Requiring that this expression be minimized with respect to the working variables then gives a set of constraint equations to determine the values of the working variables as functions of the system parameters (temperature, magnetic field, etc).

(iii) One can then determine an approximation for the critical point, by requiring that the symmetry-breaking variables display power law behaviour as the singularity is approached.

Instead of following this last step to determine the location of the critical point one can instead use the following hybrid method: use the functional expressions for values of the two-point correlation function at small separation as input to the MSA-like approximations discussed in section 3. Specifically, the CVM will give expressions for the quantities h_0 and h_1 in the equation

$$\frac{\rho h_1}{1 + \rho h_0} = \frac{z\bar{G}_0 - 1}{z\bar{G}_0} \tag{4.1}$$

as given by the MSA. We remark that it is not clear *a priori* that this method of determining the critical point will be successful, as no single consistent expansion scheme has been employed. For example, the numbers used to evaluate the RHS of (4.1) are obtained by setting $c(x)$ to zero for $|x| > a$; this type of low-density approximation is not *a priori* consistent with use of an extremely accurate value of h_1.

The algebra involved in realizing the programme outlined above has been detailed in the beautiful paper of Kikuchi [34] and will not be repeated here. We follow the notation used in that paper and merely give the results of our calculations. The variable h_1 used in section 2 to describe nearest-neighbour values of the Ising model correlation function is related to Kikuchi's variable y_1 by $h_1 = 4y_1 - 1$. If we use the lowest-order CVM, in which the only cluster in the basis set is a nearest-neighbour pair, the result is

$$h_1 = \frac{H^2 - H^{-2}}{6 - H^2 - H^{-2}} \tag{4.2}$$

with $H \equiv \exp(K_{\text{Ising}})$. This result was calculated for a two-dimensional Ising model, but at this low level of approximation, it is entirely consistent to use the relation

$$6K^{(3D)}_{\text{Ising}} = 4K^{(2D)}_{\text{Ising}} \tag{4.3}$$

noting that the Bethe approximation *per se* depends only on the combination zK, where z is the coordination number. Substituting (4.2) into (4.1) gives a critical point located at $K_{\text{crit}} = 0.779$, as compared with the value $K_{\text{crit}} = 0.8864$ given by series analysis. This is about as accurate as the value $K_{\text{crit}} = 1.099$ given by the direct Kikuchi method at the same level of approximation. An improved treatment which makes explicit use of the three-dimensional nature of the lattice [34] gives

$$h_1 = \frac{\phi^2 - 1}{\phi^2 + 6\phi + 1} \tag{4.4}$$

where the auxiliary variable ϕ is defined implicitly by

$$H^2 \equiv \exp(\tfrac{1}{2}K_{\text{LG}}) \equiv \frac{1}{\phi}\left(\frac{3\phi + 1}{\phi + 3}\right)^3. \tag{4.5}$$

Substituting (4.4) into (4.1) gives $K_{\text{crit}} = 0.926$, which is an extremely good approximation!

In order to apply the same approximation scheme to percolation models, we first develop the Kikuchi cluster approximation for bond percolation. Kikuchi [29] applied his method to site percolation by noting that it is equivalent to the zero-temperature Ising model. He treated bond percolation as site percolation on the corresponding alternate lattice. For many common lattices, e.g. the SC lattice, this requires an enlarged primitive cell and, presumably, requires including larger clusters in the basis set to give results of comparable accuracy to that obtained for site percolation. We proceed instead by calculating $K_{\text{crit}}(s)$ using the CVM for a dilute s-state Potts model, then taking the one-state limit as described in section 3. Using the Bethe approximation for the two-dimensional square lattice gives for the bond percolation threshold $p_b = 0.4226$, as compared with the exact result $p_b = 0.5$. Here we used the correspondence (3.15) between the Potts model coupling and bond probability.

We now estimate the three-dimensional bond percolation transition by using a procedure parallel to that used above for the Bethe approximation to the Ising model. First we use the direct Kikuchi procedure just described which is based on the Potts model mapping. Using the scaling $6K^{(3D)}_{\text{crit}} = 4K^{(2D)}_{\text{crit}}$ as above gives $p_b = 0.231$ for the transition point in a simple cubic lattice, as compared to the value 0.2488 given by

series methods. We now instead use the functional form for the nearest-neighbour connectedness function, as given by the Kikuchi method just described, as input to the MSA defined by (4.1). The Bethe approximation for the Potts-model variable y_1, which is the probability that a nearest-neighbour pair are in different spin states, is given by

$$y_1 = 1/[s + s(s-1)\exp(-2K)]. \tag{4.6}$$

We obtain the nearest-neighbour connectedness function h_1 for bond percolation by using the correspondence (3.8) and the relation $h_1 = 4y_1 - 1$. Using the result in the MSA as before gives a critical bond probability $p_b = 0.242$, a substantially more accurate result.

As a more involved illustration of this hybrid Kikuchi–MSA method, we consider the Wannier approximation, in which the nearest-neighbour pair and elementary plaquette, or square, are taken to be basic clusters. It seems quite difficult to use the
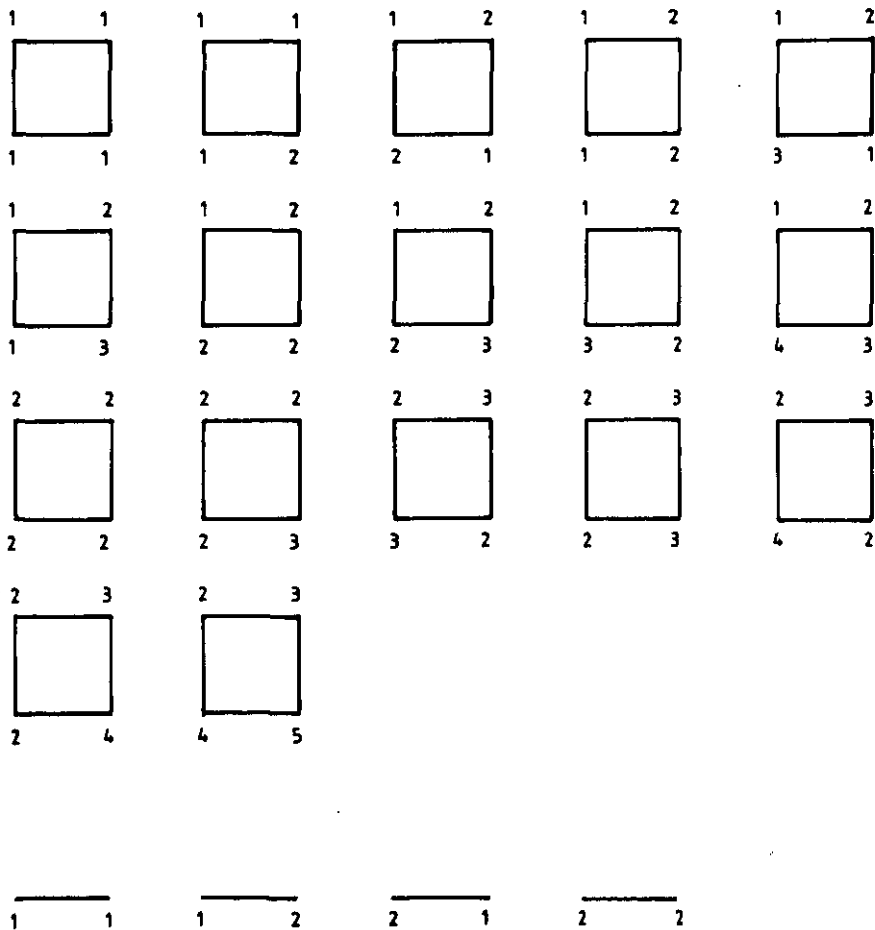

Figure 3. Configurations whose probabilities of occurrence form the working variables for the Wannier or square approximation to the properties of the s-state Potts model. By convention, '1' here denotes the symmetry-breaking state; '2', '3', etc., denote any other distinct states. The $s = 1$ limit of these variables give the two- and four-point correlation functions of bond percolation at small separation.

direct Kikuchi method described above, in which one first applies the cluster variational method to the s-state Potts model, then takes the one-state limit, as a means for locating the percolation critical point. Indeed, if the spins in the basic clusters are allowed to be in any of s states, with one of the states distinguished as the symmetry-breaking state, there are 20 different configurations of these clusters (see figure 3). Locating the critical point then involves finding the determinant of a matrix of rank 20. We note in passing that Kikuchi's method [34, 35] of realizing bond percolation as site percolation on an alternate lattice is easily seen to lead to an equally large variable set. The hybrid MSA technique developed in this section is readily applied to this model, however. Since the one-state limit of the Kikuchi method is of some interest in its own right, we describe it in the appendix. Here we simply sketch this procedure and give the result of applying it. After setting the number of states s equal to one, the values of the configuration variables in the symmetric state are quickly obtained. We derive an expression for the pair configuration variable y_{12} as a function of bond density, along with the corresponding form for h_1. Substituting this into the MSA equation (4.1) gives a percolation critical point at bond density $p_c = 0.249$. This is in remarkable agreement with the best series estimate [36], $p_c = 0.2488 \pm 0.0002$!

5. MSA-like approximations for directed percolation

In this section we apply the class of MSA-like approximations discussed in this paper to directed site and bond percolation models.

In order to gain some perspective on the strengths and limitations of the methods discussed in this paper, we use them to calculate the two-point connectedness function, and the location of the critical point, in directed percolation models. We can define these in general as follows: a distinguished direction is chosen in the space occupied by the lattice being studied. This direction may or may not coincide with one of the principle axes of the lattice. When a vector in this preferred direction is projected onto the bonds of the lattice it induces in them an allowed direction of passage. In the convention adopted here, bonds which are orthogonal to the preferred vector remain non-oriented and thus allow two-way passage or connection. Models containing a class of such bonds will then be called partly directed percolation models. This construction is motivated by one of the basic classes of applications for directed percolation models: transport through random or two-phase materials under the influence of a uniform gradient or bias field. A given lattice may then yield a number of different directed or partly directed models depending on the preferred direction chosen. In terms of MSA-like methods, these models differ from isotropic models in one basic way: random walks on the corresponding lattices either allow only a very restricted class of closed paths, or allow no such paths. The importance of this fact will be explored further when we discuss the results of this section in general terms. Here we focus on developing specific MSA-like approximations.

We may directly adapt the methods already developed to treat directed percolation as regular percolation on a lattice with peculiar connectivity [42] properties. Specifically, we make (2.9) and (4.1) the basis of our treatment. The latter will be used unchanged, while for the SC-directed lattice (with the $(1, 1, 1)$ vector the preferred direction), the equation (2.9) becomes

$$\delta_{x,0} + \rho h(x) = \frac{\Omega}{(2\pi)^3} \int \frac{e^{-ik \cdot x}}{1 - \rho c_0 - \Sigma_i \, c(x_i) \exp(k \cdot x_i)} \, d^3k \equiv G(x). \qquad (5.1)$$

Here the sum is over all sites, at positions x_i, for which $c_i \neq 0$. In general, directed percolation models will have two correlation lengths, both of which become infinite at the critical point [37]. We focus here on the value predicted by the MSA for the critical point. We calculate nth-order approximations as follows:

(i) We assume that the n values of $c(x)$ corresponding to nearest-neighbour, next-nearest neighbour, etc., separation are non-zero; for larger separations x we assume $c(x) = 0$. The non-zero values c_i are related by the random-walk representation (5.1) to non-zero values of step fugacities w_i by

$$w_i = c_i. \tag{5.2}$$

Here w_1, w_2, etc., are fugacities for steps to nearest-neighbour, next-nearest neighbour, etc., sites. We have used the fact that $c_0 = 0$ for this model; this can be seen by setting $x = 0$ in (5.1).

(ii) One then solves n equations of form (4.1) for the step fugacities w_i as functions of the (site or bond) density. Here we use explicit, exact formulae for both the connectedness function h_i and the random-walk generating function zG_i. These are readily found because the directed random paths between any pair of points which contribute to these functions are self-avoiding walks, i.e. they lack loops. Also, the number of such walks is small.

(iii) Substituting the exact fugacities $w_i(\rho)$ into the criticality condition $\Sigma_i\, w_i = 1$ then gives a polynomial equation whose smallest positive root is the critical density.

The critical densities given by successive approximations of this type are listed in table 2. The site percolation estimates seem to converge rapidly; however, for both site and bond problems, the resulting critical density to fifth order remains lower than the simulation value by about 8%.

Table 2. Approximations to directed percolation thresholds given by (3.18). The slow convergence is believed to be a result of the failure of this scheme to include recurrence in the underlying random-walk representation (see discussion in section 7). The results labelled 'Series' are from [37].

Order of approximation	Bond percolation	Site percolation
1	0.333	0.333
2	0.348	0.395
3	0.352	0.396
4	0.356	0.396
5	0.362	0.396
(Series)	0.384	0.432

6. Limitations of the MSA and directions for further research

In this section, we analyse possible reasons for the failure of MSA-like methods to yield highly accurate percolation thresholds for some systems, despite their great success for others.

Why do MSA-like methods give substantially better threshold values for bond percolation models than for site percolation models? Of course, the extension of MSA-like methods in the former case is better motivated than in the latter case; this was the purpose of our development of the Potts model formalism in section 3. But

we need a more basic understanding to extend these methods further. Here we will explore two possible elements in such an understanding.

The dominant singularity in the Mayer expansion of mean cluster size, and other physical quantities that describe bond percolation models, is the physical percolation threshold. This is not true in general for site percolation models; their dominant singularity tends to be located at a negative real value of density. Dominance by unphysical singularities has also been found in the series expansions of directed site models [37].

We have no general argument that MSA-like approximations will yield a real, positive density as the dominant singularity. However, this is found to be the case with all the approximations studied in this paper. The dominant singularity in the anti-ferromagnetic lattice Potts model lies on the negative real axis. In the MSA, the Potts model for negative density is mapped onto bond percolation at positive density; thus, in the MSA, the dominant singularity of bond percolation occurs at a positive, physical density. We observe the same fact in the MSA-like approximations studied in section 5. If one plots the singularities of the mean cluster size, which are just the zeros of the polynomial equation

$$\rho \hat{c}(k=0, \rho) = 1 \tag{6.1}$$

one always finds the dominant singularity at a physical density. The unphysical singularities associated with site percolation also cause difficulties in applying other standard methods for studying phase transitions. High-precision treatment of such structures via approximations of MSA type is thus an open problem.

The slow convergence exhibited by the MSA for three-dimensional directed problems can be understood in two complementary ways. We briefly describe both of them. In the direct form of the MSA described in section 5 for directed percolation models, the connectedness function is represented as a generating function for directed random walks. The MSA, roughly speaking, uses the balance between random walks that return to their starting point and those that do not to capture the balance between the short-range and long-range behaviour of $g_c(x)$ at criticality. In directed models in which all walks lack recurrences, this balance is missing because only short walks can contribute to the approximations for $g_c(x)$ at small separation. The argument to be discussed next suggests that three dimensions might offer special difficulties for any use of the MSA to study the properties of directed systems. However, preliminary work with the method of section 5 shows that it displays the same convergence difficulties in four dimensions.

Equivalently, one can reformulate the problem of calculating the percolation threshold in terms of random walks with recurrence, but in $(d-1)$ dimensions. If a directed three-dimensional percolation cluster is projected onto the plane perpendicular to the preferred direction, each site can be identified with a two-dimensional vector $r_\perp$, its position in the perpendicular plane with respect to the origin of that cluster. Then define [37]

$$S(\bar{r}_\perp) = \int \mathrm{d}r_\parallel \, g_c(r_\parallel, r_\perp = \bar{r}_\perp)$$

$$= \int \mathrm{d}k_\perp \exp(-\mathrm{i}k_\perp \cdot \bar{r}_\perp) \hat{g}_c(k_\perp, k_\parallel = 0) \tag{6.2}$$

to be the expected number of sites contained in the cluster and located at lateral positions $\bar{r}_\perp$. Proceeding as in section 3 then shows that $S(\bar{r}_\perp)$ is given by the generating

function of a random-walk process in $(d-1)$ dimensions. This process occurs, in general, on a directed lattice (for the three-dimensional SC lattice the corresponding process occurs on the two-dimensional directed cyclic triangular lattice [38]), but involves random walks with non-zero probability of return to the origin. However, this formulation shows that the MSA describes a directed three-dimensional process in terms of a two-dimensional process. Since the MSA is well known to be inappropriate for two-dimensional problems (again, because of the recurrence properties of two-dimensional random walks), this gives another view of the failure of the MSA in this case. From this analysis, however, one sees that the MSA might well give accurate critical densities for higher-dimensional (>3) directed percolation.

7. Conclusions

The MSA approach to site percolation has been successfully extended to both bond percolation and general site–bond percolation. The bond percolation threshold given by this method is found to coincide with an analytic estimate already shown to be of high accuracy. For the general site–bond percolation model on the SC lattice, the percolation locus calculated from this approximation agrees quite well with that given by simulation. Better agreement will require a general, reliable method for treating site percolation models, possibly using the corresponding Potts model mapping [27].

A class of approximations of MSA type have been applied to directed site and bond percolation models. These approximations give moderate accuracy, but will require basic improvements to give highly accurate predictions. Some reasons for this have been identified.

A major advantage of this approach to percolation is that the resulting integral equations can be solved analytically to give the connectedness function $g_c(x_{12})$. Summing this function over all possible separation vectors x_{12} then gives the mean cluster size. The results described in this paper can be generalized in a number of directions without giving up this advantage. For example, the bond probability, which in this paper was taken to be non-zero only for particles with nearest-neighbour separation, can be taken to have certain, non-trivial, long-range forms while still allowing exact solution for the connectedness function [5].

It would be valuable to have efficient computational procedures for the accurate determination of $g_c(x_{12})$ in a general correlated percolation problem. The hybrid procedure discussed in section 4, in which the Kikuchi method is used to calculate the short-range values of $g_c(x_{12})$ and used subsequently in the MSA, shows great promise in preliminary studies reported here. It would be useful to find a direct Kikuchi approximation for bond percolation, so as to eliminate the added algebraic complexity introduced by the Potts model map, if this is possible.

Also, in some models it may be necessary to use clusters substantially larger than those tractable by analytic means. For these models, an analogue to the numerical methods used in the phenomenological renormalization group would be valuable.

These matters are presently under study.

Appendix. Four-site Kikuchi approximation for h_1

In this appendix, we sketch the Wannier, or four-site, approximation for bond percolation on the sc lattice.

In the Wannier, or four-site, approximation, the bond and square composed of nearest-neighbour sites are chosen as the set of small clusters used as a basis for building up correlations. For a general, s-state Potts model, there are 20 different configurations of the spins in these clusters. These are shown in figure 3. The variables giving the probability of occurrence of each site, bond and square configuration are denoted by x_i, y_{ij} and z_{ijkl}, respectively, where the subscripts give the values of the site variables involved. In terms of these variables, the Kikuchi method gives, for the free energy of the system,

$$\beta F = (\tfrac{1}{2}z)K \sum_{i,j} y_{ij}(1 - \delta_{ij})$$

$$-\left\{ 9 \sum_{ij} (y_{ij} \ln y_{ij} - y_{ij}) - 7 \sum_i (x_i \ln x_i - x_i) - 3 \sum_{ijkl} (z_{ijkl} \ln z_{ijkl} - z_{ijkl}) \right\}$$

$$- C\left(\sum_i x_i - 1 \right) - \sum_i D_i \left(\sum_j y_{ij} - x_i \right) - \sum_{ij} E_{ij} \left(\sum_{kl} z_{ijkl} - y_{ij} \right). \tag{A1}$$

Here z is the coordination number and K is the Potts coupling constant. The first term in this expression is the energy per spin, the term in braces gives the entropy per spin, and the last three terms incorporate constraints due to the normalization of variables.

The expression (A1) is minimized by meeting the conditions

$$7 \ln x_i - C + D_i = 0 \tag{A2}$$

$$\tfrac{1}{2}zK(1 - \delta_{ij}) - 9 \ln y_{ij} - D_i + E_{ij} = 0 \tag{A3}$$

$$\sum_{4\,\mathrm{cp}} (3 \ln z_{ijkl} - E_{ij}) = 0 \tag{A4}$$

where the sum in the equation (A4) is over the four cyclic permutations of $(ijkl)$. It is not difficult to solve these equations in the symmetric phase. In the limit $s \to 1$, the variables with all indices equal take the value unity; in this limit they give the correlations of a non-interacting spin model. The one-state limit of variables whose indices are not all equal is also well defined, however, and gives the correlation functions of bond percolation [7, 8]. For example, the one-state limit of y_{12} gives the nearest-neighbour value of the blocking function; this is the lattice analogue of (3.8). This quantity is given by

$$y_{12}^3 = x^4/(1 - p_b) = (3x^2 - 3x^3 + x^4)^3 \tag{A5}$$

where the auxiliary variable $x = \exp(\tfrac{1}{12}E_{12})$ with E_{12} the Lagrange multiplier in (A1). Equation (A5) determines the nearest-neighbour correlation function $h_1 = 1 - y_{12}$ as a function of the bond density p_b. Substituting this into (2.19) gives, for the bond percolation threshold in the sc lattice, $p_b = 0.249$, which is in excellent agreement with the series estimate $p_b = 0.2488 \pm 0.0002$ [36].

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