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1986 J. Phys. A: Math. Gen. 19 2841

(http://iopscience.iop.org/0305-4470/19/14/020)

J. Phys. A: Math. Gen. 19 (1986) 2841-2854. Printed in Great Britain

Lattice models of aspects of firn closure: I. Percolation on the interstices of the BCC lattice

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Received 12 July 1985, in final form 30 December 1985

Abstract. The use of the percolation model to describe the age distribution of air bubbles trapped in polar ice is discussed. An earlier Monte Carlo simulation of bubble trapping defined as a bond percolation process on the interstices of a BCC lattice is checked against series analysis. A description is given of the way in which high-density series for bond percolation on bipartite lattices can be obtained by using the definition of percolation as the $q \to 1$ limit of the Potts model and applying the method of partial generating functions.

1. Introduction

Recently, the percolation model from lattice statistics has been used to describe the age distribution of air bubbles trapped in polar ice (Enting 1985, Stauffer *et al* 1985). The determination of the distribution of trapping times is needed if observed concentrations of minor atmospheric constituents (e.g. CO_2, CH_4) are to be used to reconstruct a history of changes in atmospheric composition over the last few centuries. In terms of the notation used by Enting (1985) the trapping distribution $R(z)\,dz$ is the amount of gas trapped in an ice layer during the period z to $z+dz$ years after the original snow was deposited. $R(z)$ is normalised by

$$\int_0^\infty R(z)\,dz = 1 \tag{1}$$

so that $R(z)$ is the trapping rate expressed as a proportion of total gas trapped. From the definition of $R(z)$ it follows that $q(z)$, the concentration of any constituent occurring in bubbles in an ice layer that is z years old, is related to $c(z')$, the atmospheric composition z' years ago, by

$$q(z) = \int_0^z R(z-z')c(z')\,dz'. \tag{2}$$

The static geometric aspects of bubble trapping can be modelled using percolation theory by assuming that connecting channels close with a probability that increases with the age z of the layer. The proportion of gas that is not trapped is the proportion still connected to the atmosphere by open channels. This is identified with the proportion of sites connected to an infinite cluster of open channels, i.e. to a cluster through which air percolates from the atmosphere. This is $P(z)$, the percolation probability expressed in terms of the age z and so the cumulative proportion trapped is $1-P(z)$ and the trapping rate $R(z)$ is the derivative $-P'(z)$. The relation between z, the age of the ice, and the bond closure probabilities must be determined empirically.

0305-4470/86/142841+14$02.50

Two initial studies of bubble trapping used bulk three-dimensional percolation as the basic model, thus identifying the percolation transition with the transition from firn (i.e. permeable layers of sintered snow grains) to impermeable ice layers. Stauffer *et al* (1985) considered bond percolation on the interstitial sites of a BCC lattice and performed Monte Carlo simulations in order to estimate the critical point. Enting (1985) invoked universality arguments in order to discuss the dominant singularity occurring in equation (2). If a percolation model is used then equation (2) becomes

$$q(z) = -\int_{z-z_c}^{z} P'(z-z')c(z')\,\mathrm{d}z' \qquad z \geqslant z_c \tag{3a}$$

or

$$q(z) = -\int_{0}^{z} P'(z-z')c(z')\,\mathrm{d}z' \qquad z \leqslant z_c. \tag{3b}$$

Enting (1985) pointed out that, since $P'(z)$ is expected to diverge at z_c as $(z_c - z)^{\beta-1}$, the deconvolution involved in solving the integral equation (3*a*) should be less poorly conditioned than most geochemical inversion problems.

The use of bulk three-dimensional percolation probabilities to model bubble trapping is, of course, only an approximation and a number of refinements to the model should be investigated further. Many of the refinements involve special problems that have been studied individually in the past. Among the aspects of bubble trapping that are in need of further study in order to produce a refined model are diffusion effects, crossover effects, the effects of the vertical density gradient in the firn and the role of critical fluctuations. These matters have been discussed in greater detail by Enting (1986).

The main aim of the present paper is to analyse series expansions for bond percolation on the interstices of a BCC lattice as a crosscheck on the Monte Carlo analysis presented by Stauffer *et al* (1985). In addition it is pointed out that the most appropriate percolation model for bubble trapping is not the conventional bond percolation model considered by Stauffer *et al* but is rather the percolation model obtained from the $q \to 1$ limit of the q-state Potts model.

The layout of the remainder of this paper is as follows. Section 2 describes the Potts model formulation of the bond percolation problem and the structure of high-field/low-temperature series. Section 3 gives an explicit technique for series derivation using partial generating functions. This is a modification of the techniques described by Enting (1975) which generalised the so-called 'code method' of Sykes *et al* (1965). The series analysis is presented in § 4. Section 5 compares the results of the series expansion to the Monte Carlo results of Stauffer *et al* (1985).

2. Percolation and the Potts model

There have been a number of discussions of the representation of bond percolation in terms of the Potts model from statistical mechanics (e.g. Fortuin and Kasteleyn 1972, Wu 1978). The overall result is that the lattice statistics of bond percolation can be obtained from the q-state Potts model. The percolation model that is generated in this way describes the statistics of clusters of sites that may be connected by randomly occurring bonds. The conventional formulation of bond percolation considers the statistics of clusters of bonds. The order parameter obtained from the Potts model is

a percolation probability which is the probability that a given site is part of an infinite cluster, rather than the more common definition that the percolation probability is the probability of a given bond being part of an infinite cluster.

Obviously, since infinite clusters of sites will have an infinite number of bonds (and vice versa), both forms of the percolation probability will go to zero at the same p_c on any given lattice. Universality would indicate that all critical exponents will be the same in each case, and the equality of the exponent β has been proved by Blease *et al* (1976).

As well as lending itself readily to the series derivation techniques described below, the percolation probability derived from the Potts model is the most natural form to use in modelling bubble trapping. In this representation the sites represent cavities in which gas can be trapped and the bonds represent the narrow pathways connecting these cavities. As the density of the firn increases it is the narrow pathways (bonds) that close randomly while the amount of trapped gas is dominated by the number of cavities (sites). Thus the statistics of bubble trapping correspond to the statistics of number of sites connected by randomly closed bonds as given by the $q \to 1$ limit of the Potts model.

A rigorous justification of the use of the Potts model approach to derive series expansions for percolation is a very delicate problem. There are three limits involved: the $N \to \infty$ thermodynamic limit, the $q \to 1$ limit of the Potts model to give percolation and the $H \to 0$ limit involved in defining an order parameter. It is well known that the N = number of sites $\to \infty$ and H = ordering field $\to 0$ limits cannot be exchanged without changing the results. However, the question of whether the $q \to 1$ limit can be interchanged with the other limits has not, to the author's knowledge, been fully discussed particularly in the context of deriving high-field expansions.

The Potts model Hamiltonian is written as

$$\mathcal{H}/kT = -K \sum_{\langle ij \rangle \in E} \delta(\sigma_i, \sigma_j) - L \sum_{i \in V} \delta(\sigma_i, 0) \tag{4}$$

where σ_i is a q-state variable with values $0, 1 \ldots, q-1$ and

$$\delta(a, b) = 1 \qquad \text{if } a = b \tag{5a}$$

$$= 0 \qquad \text{otherwise.} \tag{5b}$$

The first sum in (4) is over the set E of edges of the lattice and the second sum is over V, the set of N sites. The Potts model partition function Z is defined by

$$Z(q, K, L) = \sum_{\sigma_1=0}^{q-1} \ldots \sum_{\sigma_N=0}^{q-1} \exp(-\mathcal{H}/kT). \tag{6}$$

Wu (1978) shows that the percolation probability can be rewritten as

$$P(p) = 1 + \frac{\partial}{\partial L} \frac{\partial}{\partial q} \left(\lim_{N \to \infty} N^{-1} \ln Z(q, K, L) \right) \Bigg|_{q=1} \tag{7}$$

if $Z(q, K, L)$ is defined for non-integer q in terms of the random-cluster model (Fortuin and Kasteleyn 1972) which has a graph generating function $Z(q, K, L)$ which is equal to that defined by equation (6) for integer q. In equation (7) the bond occurrence probability p is given by

$$p = 1 - u = 1 - \exp(-K). \tag{8}$$

The Potts model partition function Z and its logarithm have high-field expansion in terms of $\mu = \exp(-L)$. The expansion for $\ln(Z)$ has been discussed by Enting (1974a, b). The coefficients of μ^n are finite polynomials in u and q, with the maximum powers being $u^{n\nu}$ and q^n where ν is the lattice coordination number. For the present we assume that the general random-cluster model has an expansion with the same properties, and if this is so then the small μ expansion for the random-cluster model can be obtained simply by substituting non-integer q values into the general q expansion for the Potts model. (A full proof of the validity of using this assumption would seem to require a demonstration that the $q \to 1$ and $N \to \infty$ limits can be validly exchanged. For finite graphs, the reinterpretation of Potts model expansions as random-cluster expansions must be correct since the random-cluster generating function is a finite polynomial in μ, u, q that agrees with the Potts model for all positive integers q.)

The final points to note are that the high-field expansion is an expansion about the fully ordered state which is the sole allowed state of the one-state Potts model, i.e. the high-field expansion is an expansion for $\tilde{Z}$ where

$$Z(q, K, L) = Z(1, K, L)\tilde{Z}(q, K, L). \tag{9}$$

Thus

$$\frac{\partial}{\partial q} \ln Z \bigg|_{q=1} = \frac{\partial}{\partial q} \ln \tilde{Z} \bigg|_{q=1} = \frac{\partial}{\partial q} \tilde{Z} \bigg|_{q=1} \tag{10}$$

and, since $\partial/\partial L = -\mu\, \partial/\partial \mu$,

$$P(p) = 1 - \mu(\partial/\partial\mu)\tilde{Z}. \tag{11}$$

3. Series expansions from partial generating functions

As indicated in the introduction, the aim of this paper is to study series expansions for the percolation probability of the bond percolation model (as derived from the Potts model) on the interstitial sites of a BCC lattice. The lattice structure is that of the silicon atoms in the ultramarines $(Na_{4+x}(Si_{24}Al_xO_{48})(X_2)_2)$ (Krebs 1968). The lattice is shown in figure 1. It has coordination number $\nu = 4$. For the purposes of deriving series expansions the most important property is that it is bipartite, dividing into two equivalent sublattices, so the techniques developed for the Ising model by Sykes *et al* (1965) and described for the general-q Potts model by Enting (1975) can be applied.

The derivation of the series involves a sequence of steps that is outlined here.

3.1. The existence of high-field expansions for Z

As indicated in the previous section, $Z(q, K, L)$ can be expanded in powers of $\mu = \exp(-L)$. For the Potts model, this expansion has a graphical representation in terms of perturbed sites with the power of μ being given by the number of perturbed sites.

3.2. The low-temperature grouping

The coefficients of μ^n are polynomials in u of degree νn where ν is the coordination number. In two or more dimensions the lowest power increases with n and so the

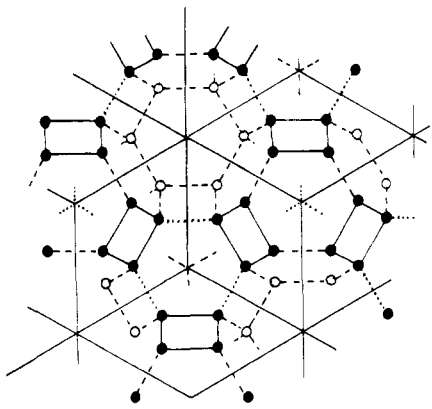

Figure 1. Ultramarine lattice. The sites are the interstitial sites of a BCC lattice. The lattice is cut away along faces of the underlying simple cubic lattice which is included to aid the interpretation. The full lines and full circles of the ultramarine lattice lie on the exposed cube faces whose boundaries are also full lines. The open circles and broken lines (on both cubic and ultramarine lattices) lie behind the exposed cube faces and the dotted lines lie in front of the exposed cube faces.

high-field expansion can be regrouped as a low-temperature expansion. The minimum power is given by $n\nu - 2e_{max}$ where e_{max} is the maximum possible number of edges that can occur in any graph of n vertices that can be embedded in the lattice. For $n = 1, 2, \ldots, 12$ the minimum powers for the ultramarine lattice are 4, 6, 8, 8, 10, 12, 12, 14, 16, 16, 18 and 18 respectively. Examples of graphs that lead to these minimum powers are given in figure 2. From this grouping it will be seen that a combination of

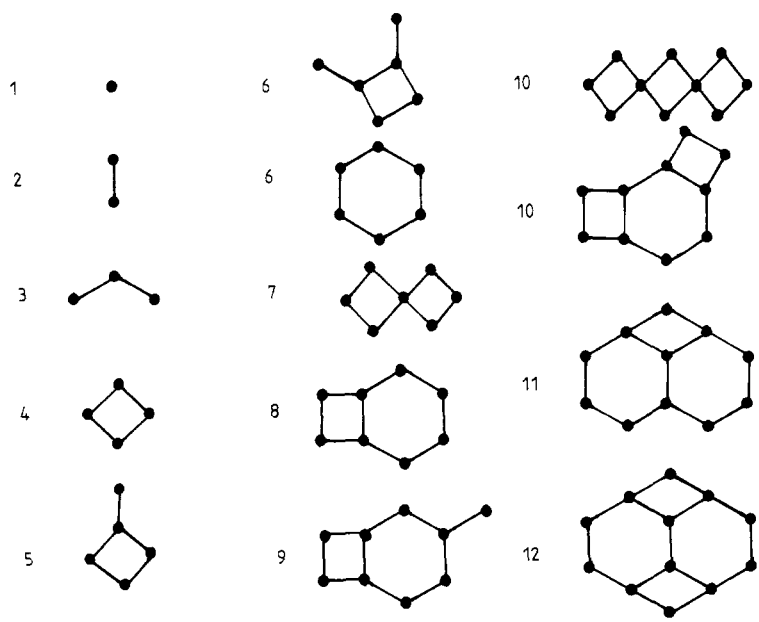

Figure 2. Graphs that define the temperature grouping of the series. For each number of sites, n, no other strong subgraph of the ultramarine lattice has more bonds.

a full expansion to μ^7 combined with explicit consideration of a small number of graphs for μ^8 will give series through to u^{15}.

3.3. Connected graph expansions

The high-field expansions represent perturbations of groups of sites from the zero state into some of the other $q-1$ states. Thus, for any particular perturbation, $(q-1)^\gamma$ equivalent perturbations can be constructed by applying independent cyclic permutations separately to each of the γ connected clusters. (For many perturbations there are additional equivalent perturbations but these can be obtained by applying additional permutations independently of the cyclic permutations and so the combinatorial factors have a factor of $(q-1)^\gamma$.) If the expansion of Z has its terms with factors $(q-1)^\gamma$ (with integer $\gamma \geq 1$) then only those terms with $\gamma = 1$ (i.e. perturbations of connected sites) will contribute to the expansion of $\partial Z/\partial q$ at $q=1$. A consequence of this requirement is that the coefficients of μ^n reduce from being polynomials of degree νn in u for general q down to being of degree $(\nu-1)n+1$ for the $q \to 1$ limit. Furthermore these polynomials are the appropriate generalisation (for the modified bond percolation model) of the perimeter polynomials defined for the more conventional site and bond problems by Sykes and Glen (1976) and Sykes *et al* (1981) respectively. The coefficient of μ^n will thus have $p^{n-1} = (1-u)^{n-1}$ as a factor. This property serves both as a check on the derivation of the expansions in powers of u and as a way of deriving low-density expansions in powers of p.

3.4. Integer coefficients for the percolation problem

For lattices in which all sites are equivalent (and in particular for the ultramarine lattice) the percolation probability has an expansion with integer coefficients. To see this we note that the standard definition of the percolation probability would be

$$P = 1 - \sum_g \mu^{v(g)}(1-u)^{e(g)} u^{n\nu - 2e(g)}$$

where the sum is over all finite graphs g representing clusters of sites containing an arbitrarily chosen origin. It should be noted that, unlike many other simpler lattices, the expansion for $\tilde{Z}$ on the ultramarine lattice involves fractional coefficients.

3.5. Two-field expansions

The method of partial generating functions devised by Sykes *et al* (1965) and extended to the general-q Potts model by Enting (1975) applies to lattices which can be divided into two equivalent sublattices A and B such that all bonds on the original lattice connect A sites to B sites. In such cases, the partition functions are generalised by having distinct fields L_A and L_B applying on the two sublattices. This leads to a high-field expansion of the form

$$\tilde{Z}(q, K, L_A, L_B) = \sum_m \sum_n \mu_A^n \mu_B^m \lambda_{mn}(q, u).$$

The utility of this approach is that for small m the full sum over n can be performed to give

$$F_m(\mu_A, q, u) = \sum_n \mu_A^n \lambda_{mn}(q, u).$$

If the F_m are known up to some order M, the symmetry $\lambda_{mn} = \lambda_{nm}$ can be used to obtain all λ_{mn} for $m+n \leqslant 2M+1$ and setting $\mu_A = \mu_B$ allows $\tilde{Z}(q, K, L)$ to be obtained through to μ^{2m+1}.

The $F_m(\mu_A, q, u)$ are expressed in terms of the sets of m perturbed sites on the set of B sites which is called the shadow lattice. Two shadow lattice sites are connected if and only if they have a common neighbour on the A lattice. With this definition of connectivity it will be seen that B sites of a graph that is connected on the original lattice will be connected on the shadow lattice and so, from § 3.3, $\partial Z/\partial q$ at $q=1$ can be calculated from a reduced $\tilde{F}_m(\mu_A, q, u)$ which only includes contributions from connected shadow lattice graphs. Furthermore the graphs will make contributions to $Z(q, K, L)$ of the form $(q-1)\phi(q, u, \mu_A)$. Differentiating with respect to q and setting $q=1$ shows that the corresponding contribution to $\partial Z/\partial q$ at $q=1$ is $\phi(1, u, \mu_A)$. Thus for the percolation model $q=1$ can be substituted directly into the factors f_i given by Enting (1975). (The one exception is for F_0 where there are no B lattice sites to give a $(q-1)$ factor.)

3.6. The series expansion

The final result of this analysis is that we can write

$$\left.\frac{\partial Z}{\partial q}\right|_{q=1} = \tfrac{1}{2}N \sum_{m,n} \mu^{m+n} \tilde{\Lambda}_{mn}$$

where the $\tilde{\Lambda}_{mn}$ are derived from $\tilde{F}_m$ which are formally

$$\tilde{F}_m = \sum_{n=0}^{\infty} \mu_A^n \tilde{\Lambda}_{mn}$$

and which can be constructed explicitly as sums over shadow lattice graphs as described by Enting (1975).

Enting gives

$$F_0 = \ln[1+(q-1)\mu_A u^z]$$

whence $\tilde{F}_0 = \mu_A u^z$. The higher-order $\tilde{F}_m$ are expressed as sums over all connected sets of perturbed sites on the shadow lattice

$$\tilde{F}_m = \sum_g f_i^{w(i,g)}$$

where the index i denotes a type of perturbed element in cluster g and $w(i, g)$ is the number of times such an element occurs in cluster g.

From Enting (1975) the various elements and the f_i for Potts model perturbations (evaluated at $q=1$) are

$$f_2 = 1 + \mu u^{\nu-2} - \mu u^{\nu-1}$$

for each A site neighbouring only one perturbed B site;

$$f_3 = 1 + \mu u^{\nu-4} - \mu u^{\nu-2}$$

for each A site neighbouring exactly two perturbed B sites in the same perturbed state;

$$f_4 = 1 + 2\mu u^{\nu-3} - 2\mu u^{\nu-2}$$

for each A site neighbouring two B sites in different perturbed states;

$$f_5 = 1 + \mu u^{\nu-6} - \mu u^{\nu-3}$$

for each A site neighbouring three B sites in the same state;

$$f_6 = 1 + \mu u^{\nu-5} + \mu u^{\nu-4} - 2\mu u^{\nu-3}$$

for each A site neighbouring three B sites, two of which are in the same state;

$$f_7 = 1 + 3\mu u^{\nu-4} - 3\mu u^{\nu-3}$$

for each A site neighbouring three B sites in distinct states.

Terms involving the same powers of the f_i can be grouped to give expansions of the form

$$m\tilde{F}_m = \sum_n C_n f_2^{n_2} \ldots f_7^{n_7}$$

which is denoted

$$m\tilde{F}_m = \sum_n C_n \langle n_1, n_2, \ldots, n_6 \rangle$$

with n_1, which is always 0 here, included for consistency with previous descriptions. The expansions of $\tilde{F}_1$ to $3\tilde{F}_3$ are given in the appendix, with trailing zeros in the $\langle\ \rangle$ factors truncated. The factor m is included in the definition of the C_n since this gives integer coefficients.

The shadow lattice graphs and their weights (without the factor m) are shown in figure 3. The double lines represent bonds between two B sites with two common A neighbours while the single lines connect B sites with only one common A neighbour. The shaded triangles have an A site which is a common neighbour of the three (B-site) vertices of the triangle.

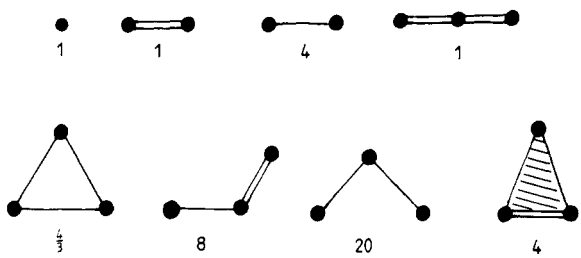

Figure 3. Counts for graphs of up to three sites on the shadow (B) lattice of the ultramarine lattice. Single lines connect B sites with one common A neighbour and double lines connect B sites with two common A neighbours. The three B sites in the shaded triangle have a common A neighbour.

In order to generate the 'codes' in the appendix, the $(q-1)^m$ decorations of each graph must be considered. As indicated earlier, there are also a number of μ^8 contributions that must be considered in order to obtain the full series to order u^{15}. The relevant graphs are shown in figure 4, together with their counts on the ultramarine lattice. The fourth graph contributes to $\tilde{\Lambda}_{35}$ and so its contribution will be obtained correctly from $\tilde{F}_3$ but the other three contribute only to $\tilde{\Lambda}_{44}$ and so must be considered explicitly. The leading contribution (of order $q-1$) for each graph is $u^{14}\mu^8$ and so the graphs

combine to contribute $14u^{14}\mu^8$ to $\tilde{Z}$ and $-112u^{14}\mu^8$ to P. The first and third graphs have additional contributions with factors $(q-1)(q-2)$ corresponding to perturbations into two different Potts model states. If the break between the two states occurs across the unique cutting line in each graph then the contributions are $(q-1)(q-2)\mu^8u^{15}$ so the graphs contribute $-10\mu^8u^{15}$ to $\tilde{Z}$ and $80\mu^8u^{15}$ to P. All other perturbations of any of the three graphs give higher powers of u.

Combining these corrections with the expansion of the partial generating functions from the appendix gives

$$P(p=1-u)=1-u^4-4u^6+4u^7-20u^8+36u^9-106u^{10}+244u^{11}-646u^{12}$$
$$+1572u^{13}-3978u^{14}+9708u^{15}\ldots.$$

The derivation of the series for $P(p)$ can be immediately extended to the derivation of series for $S(p)$, the mean size of finite clusters, since, from Wu (1978),

$$S(p)=\frac{\partial^2}{\partial L^2}\frac{\partial}{\partial q}\left(\lim_{N\to\infty} N^{-1}\ln Z(q,K,L)\right)_{q=1}$$

The resulting high-density series is

$$S(p=1-u)=u^4+8u^6-8u^7+62u^8-108u^9+426u^{10}-996u^{11}+3170u^{12}$$
$$-8092u^{13}+23\,222u^{14}-60\,208u^{15}+\ldots.$$

Regrouping the perimeter polynomials (i.e. coefficients of μ^n) gives the low-density series

$$S(p)=1+4p+12p^2+36p^3+98p^4+280p^5+764p^6+2112p^7+\ldots.$$

The last term has been deduced by exploiting the fact that the low-density expansion for $P(p)$ must be identically zero.

4. Series analysis

The high-density series derived in the previous section are relatively short, extending only to u^{15}. While this is longer than, for example, the three-state square lattice Potts

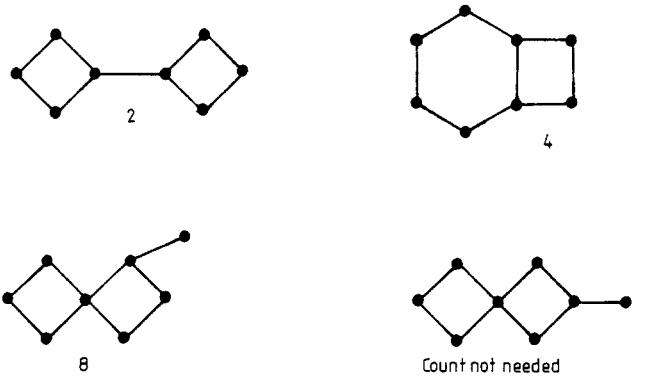

Figure 4. Graphs on the ultramarine lattice with eight sites and nine bonds. The first three (whose counts are shown) give corrections to the u^{14} and u^{15} terms obtained from partial generating functions up to $\tilde{F}_3$. The contribution of the fourth graph is included in $\tilde{F}_3$.

model series for which the temperature grouping is similar and which was analysed by Straley and Fisher (1973), the ultramarine series would be expected to be less regular than any corresponding square lattice series. The lattice has six sites per unit cell and so relatively high-order perturbations are needed in order to obtain a representative sample of the long range structure of the lattice from which to extract an estimate of critical behaviour.

There are however two properties that do help the analysis. The first is that an estimate of the critical exponent is available. The second is that the 'correction-to-scaling' exponent Δ_1 is near 1 (Adler *et al* 1983) and so the corrections are very nearly analytic. These properties suggest that the best estimates for the critical point will be obtained by constructing Padé approximants to $P^{1/\beta}$ and looking for the smallest real zero of the numerator.

The exponent β was taken to be 0.454, based on the work of Gaunt and Sykes (1983). The results of the Padé approximant analysis are shown in table 1. The first column gives the order of the approximant that was fitted to $P(u)^{1/0.454}$. The second column is the smallest positive real zero of the numerator. These values are estimates of u_c. The final column gives the value of the smallest positive real zero of the denominator. It will be seen that the smallest values of the u_c estimates are associated with an additional pole in the approximant just beyond the physical singularity. The third column gives the residue of the approximant at the physical singularity. The fourth column gives the smallest negative zero of the numerator. This seems to be a well defined singularity (as might be expected given the regular alternation in sign of the original series). However the zero is almost always followed closely by a pole which suggests that the approximants are attempting to model a singularity that does not follow the $(u_c - u)^\beta$ behaviour that was assumed for the physical singularity.

It will be seen that there are two distinct interpretations concerning the physical singularity that could be placed on the results in table 1. The first is that the critical behaviour is described by a simple power law and the critical point is $u_c = 0.61 \pm 0.01$. The second interpretation is that the singularity is at $u_c = 0.580 \pm 0.015$ but with singular behaviour that is more complicated than a simple power law so that the Padé approximants represent this more complicated behaviour with an additional pole just beyond the physical singularity. The significance of this second possibility is that the critical probability would then be in agreement with the Monte Carlo estimate given by Stauffer *et al* (1985).

In order to test the sensitivity of these results to the value of β that was chosen, the analysis above was repeated using values of β ranging from 0.40–0.48 in steps of 0.01 in order to cover most of the range of estimates given for various three-dimensional percolation problems by Gaunt and Sykes (1983). The behaviour of the physical singularity in each case was very regular. For each β value the [5, 5] approximant led to a complex pair. The zero of the [7, 5] approximant dropped monotonically from 0.5773 to 0.5721 as β increased from 0.40 to 0.48. The zero of the [8, 7] approximant increased from 0.5852 ($\beta = 0.4$) to 0.5864 ($\beta = 0.45$) and dropped to 0.5865 at $\beta = 0.48$. For all other approximants the position of the zero increased monotonically, changing by up to 0.0107 as β increased from 0.40 to 0.48. Where approximants are shown in table 1 as having a pole on the positive axis, this behaviour persisted when β was varied.

It is therefore apparent that the variability in the estimates of u_c arising from uncertainties in the value of β are much less than the variability shown in table 1 for a single value of β. Analysis of Padé approximants to the logarithmic derivative of P was also attempted but was unsuccessful because virtually all approximants had a complex pair of poles rather than a physical singularity.

Table 1. Results of Padé approximant analysis. $[D, N]$ denotes the order of the Padé approximant to $P(u)^{1/\beta}$ with $\beta = 0.454$. The zero on the positive real axis is an estimate of $1 - p_c$. The residues determine the critical amplitude. The zero on the negative real axis is the dominant non-physical singularity. The final column shows the pole on the positive axis that is closest to the origin, as such poles may distort the estimates of p_c. * denotes a pole–zero pair.

$[D, N]$	Zero on positive axis	Residue	Zero on negative axis	Pole on positive axis
[4, 5]	0.568	−15.81	−0.384	0.682
[5, 4]	0.576	−14.18	−0.386	0.733
[4, 6]	0.560	−17.52	−0.395	0.653
[5, 5]	Complex	—	−0.390	None
[6, 4]	0.596	−10.89	−0.415	None
[5, 6]	0.607	−9.61	−0.393	None
[6, 5]	0.620	−7.71	−0.393	None
[5, 7]	0.611	−9.01	−0.393	None
[6, 6]	0.611	−9.05	−0.393	None
[7, 5]	0.613	−8.67	−0.393	None
[6, 7]	0.608	−9.44	−0.392	None
[7, 6]	0.575	−20.20	−0.393	0.620
[6, 8]	0.604	−10.03	−0.393	None
[7, 7]	0.604	−10.13	−0.393	2.182
[8, 6]	0.606	−9.80	−0.393	None
[7, 8]	0.608	−9.38	Complex	0.114*
[8, 7]	0.586	−14.91	−0.393	0.664

The analysis of $P(p)$ was supplemented by an analysis of the series for the mean cluster size $S(p)$. The procedure that was used was to take the exponent estimate $\gamma' = 1.73$ obtained by Gaunt and Sykes (1983) and construct Padé approximants. The positions of the poles are listed in table 2 as estimates of $1 - p_c$. This analysis procedure did not produce any regular estimates of the singularity on the negative real axis and the poles representing the physical singularity were not associated with additional close poles or zeros. It will be seen that estimates of u_c are larger than the estimates obtained from the $P(p)$ series and so the discrepancy with the Monte Carlo estimates is greater.

Table 2. Results of Padé approximant analysis. $[D, N]$ denotes the order of the Padé approximant to $[u^{-4}S(u)]^{1/\gamma'}$ with $\gamma' = 1.73$. The pole on the real axis gives an estimate of $1 - p_c$. The residues determine the critical amplitude.

$[D, N]$	Pole on positive axis	Residue
[4, 4]	0.636	−0.543
[4, 5]	0.638	−0.549
[5, 4]	0.638	−0.549
[4, 6]	0.637	−0.547
[5, 5]	0.637	−0.547
[6, 4]	0.637	−0.547
[5, 6]	0.638	−0.549
[6, 5]	0.638	−0.549

For completeness the short low-density series for the mean cluster size have been analysed using the ratio method. The results are given in table 3. The use of ratios of successive terms gives a regular oscillation similar to the behaviour of Ising model susceptibilities series in which there is an antiferromagnetic singularity. This oscillation

Table 3. Ratio method analysis of the low-density expansion of the mean cluster size, $S(p) = \Sigma\, s_n p^n$. The last two columns are estimates of p_c, assuming that the critical exponent is $\gamma = 1.73$.

n	s_n	$f_n = 1 + 0.73/n$	$r_n^{-1} = s_{n-1}/s_n$	$\rho_n^{-1} = \sqrt{s_{n-2}}/s_n$	f_n/r_n	f_n/ρ_n
0	1	—	—	—	—	—
1	4	1.7300	0.2500	—	0.4325	—
2	12	1.3650	0.3333	0.2886	0.4550	0.3939
3	36	1.2433	0.3333	0.3333	0.4144	0.4144
4	98	1.1825	0.3675	0.3499	0.4344	0.4138
5	280	1.1460	0.3500	0.3586	0.4011	0.4110
6	764	1.1217	0.3665	0.3582	0.4111	0.4018
7	2112	1.1043	0.3617	0.3641	0.3995	0.4021

has been reduced by taking the square roots of ratios of every second term. If the critical exponent is assumed to be $\gamma = 1.73$ as estimated by Gaunt and Sykes (1983) it will be seen that the ratio method gives estimates of p_c that are smaller than the estimate of $p_c = 0.42$ given by Stauffer *et al* (1985) and are in reasonable agreement with the Padé approximant analysis in table 1. Using γ values of 1.64 and 1.74 to cover the range of values found by Gaunt and Sykes (1983) for the simple cubic bond problem makes only small changes to the ratio method estimates which remain significantly smaller than the estimates by Stauffer *et al.*

5. Discussion

There are two main aspects of this paper. The first is the presentation of a technique for deriving series expansions for bond percolation by using partial generating functions. (The results of an earlier unpublished application (by the present author) of this technique in the derivation of series along the 'critical isotherm' of the square lattice bond percolation model was quoted by Gaunt and Sykes (1976).) The relative efficiency of such techniques compared with direct graph counting will depend on the particular problem and to some extent the number of terms that are required. For the ultramarine lattice, the partial generating function approach was very convenient at low orders because the small number of shadow lattice graphs involved can be counted and decorated by hand. At somewhat higher orders where computer enumeration of the graphs becomes necessary it may be most convenient to enumerate the graphs directly for the ultramarine lattice and avoid the need for decorations and algebraic expansions. However, as longer and longer series are sought it is probable that a second 'crossover' will occur where the partial generating function techniques again become the more efficient approach. The number of shadow lattice graphs should grow much less quickly than the number of graphs on the original lattice and the decorations and algebraic expansions required by the method of partial generating functions need be performed only once for each topological class.

The second aspect of this paper concerns the analysis of percolation on the ultramarine lattice. The discussion by Gaunt and Sykes (1983) indicates the extreme difficulty that has been encountered in the analysis of percolation problems. The ultramarine lattice might be expected to be particularly difficult to analyse because it has six sites per unit cell and so relatively long series may be required in order to adequately sample the lattice structure. The nature of the difficulty encountered by Gaunt and Sykes is unclear, particularly since the correction-to-scaling exponent is believed to be close to one and so the corrections should lead to functions that can be represented closely by Padé approximants. The discrepancies between u_c estimates obtained from analysing $P(p)$ and analysing $S(p)$ shows that similar problems are occurring for the ultramarine series. In view of the serious difficulties encountered by Gaunt and Sykes (1983) in analysing high-density series for the mean cluster size, the results in table 2 must be treated with considerable caution. The u_c estimates in table 1 should be regarded as more reliable, especially since they are supported by the ratio method analysis shown in table 3.

Monte Carlo techniques have been used to study a number of percolation models and very precise estimates of the critical probability have been obtained by using finite-size scaling theory to interpret the results (Sur *et al* 1976, Heerman and Stauffer 1981). Such studies have used of the order of 10^6 sites. However in the study of firn closure by Stauffer *et al* (1985) up to 8748 bonds were used and there was no indication of whether finite-size scaling was used to extrapolate the results of the simulations. It is therefore quite possible that the agreement between their estimate of $p_c = 0.42$ and the Padé approximants with the zero-pole structure on the real axis is a coincidence and of no special significance. On this assumption, the estimate of $p_c = 0.39 \pm 0.01$ is proposed as appropriate for the ultramarine lattice.

Acknowledgments

The Padé approximant analysis was performed by Dr J V Mansbridge using programs supplied by Professor A J Guttmann.

Appendix. Partial generating functions for bond percolation on the ultramarine lattice

$$\tilde{F}_1 = 1\langle 0, 4\rangle$$

$$2\tilde{F}_2 = 2\langle 0, 4, 2\rangle - 2\langle 0, 4, 0, 2\rangle + 8\langle 0, 6, 1\rangle - 8\langle 0, 6, 0, 1\rangle$$

$$\begin{aligned} 3\tilde{F}_3 = {} & 3\langle 0, 4, 4\rangle - 6\langle 0, 4, 2, 2\rangle + 3\langle 0, 4, 0, 4\rangle + 28\langle 0, 6, 3\rangle - 24\langle 0, 6, 2, 1\rangle - 36\langle 0, 6, 1, 2\rangle \\ & + 32\langle 0, 6, 0, 3\rangle + 12\langle 0, 7, 1, 0, 1\rangle - 12\langle 0, 7, 1, 0, 0, 1\rangle - 24\langle 0, 7, 0, 1, 0, 1\rangle \\ & + 24\langle 0, 7, 0, 1, 0, 0, 1\rangle + 60\langle 0, 8, 2\rangle - 120\langle 0, 8, 1, 1\rangle + 60\langle 0, 8, 0, 2\rangle. \end{aligned}$$

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