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Valences of sites in bond percolation

S G Whittington†, K M Middlemiss† and D S Gaunt‡

† Department of Chemistry, University of Toronto, Toronto, Canada M5S 1A1
‡ Wheatstone Physics Laboratory, King's College, University of London, Strand, London WC2R 2LS, UK

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Abstract. We present calculations for the fraction of sites with given valence in finite and infinite clusters in the Bethe approximation, for a lattice of coordination number Q, and compare these results with series analysis results for the bond percolation problems on the square and simple cubic lattices.

1. Introduction

Recently we have used series analysis and Monte Carlo techniques to characterise a number of properties of percolating and non-percolating clusters in site percolation problems in two and three dimensions (Middlemiss *et al* 1980, Gaunt *et al* 1980, Whittington *et al* 1980). It is now clear that the degree of ramification of a cluster depends very much on how one chooses to measure ramification, in particular whether the characterisation is based on a local or global property. Various properties have been used, such as cyclomatic index (Domb 1974, Stoll and Domb 1979, Cherry and Domb 1980), perimeter (Domb 1974, Domb *et al* 1975, Stoll and Domb 1978, Hankey 1978), valence (Gaunt *et al* 1980, Whittington *et al* 1980), radius of gyration (Stauffer 1978), backbone (Schlifer *et al* 1979) and the relative thickness of the shortest spanning walk (Middlemiss *et al* 1980).

Most of this work has been concerned with site percolation, and in this paper we consider the characterisations based on valence for the bond problem on the square and simple cubic lattices. In § 2 we discuss two alternative conventions for site occupation in bond percolation, and show that these lead to the same critical exponents. In § 3 we carry out a calculation for the interior of a Bethe lattice to obtain the distribution of valences of *sites* in percolating and non-percolating bond clusters, at all bond densities, and extract some information about critical indices in this 'Bethe' approximation. Sections 4 and 5 are concerned with series analysis results for the square and simple cubic lattices. In § 4 we discuss finite clusters and in § 5 infinite clusters. Section 6 comprises a discussion of our results.

2. Mean valence of sites in bond clusters

In discussing bond percolation there is a possible ambiguity in defining when a site is occupied. One possibility is to regard *all* lattice sites as being automatically occupied whether or not a bond is incident on that site. In this case it is necessary to consider sites

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having zero valence, i.e. belonging to clusters with zero bonds. For a lattice of coordination number Q, the mean valence at bond density p, $\langle v_0(p)\rangle_E$, of a site in any cluster (i.e. one with zero bonds, a non-zero but finite number of bonds, or an infinite number of bonds) is given by

$$\langle v_0(p)\rangle_E = \sum_{i=0}^{Q} i\binom{Q}{i}p^i q^{Q-i} \Big/ \sum_{i=0}^{Q}\binom{Q}{i}p^i q^{Q-i}$$
$$= Qp \tag{2.1}$$

where $q = 1-p$. This result is formally identical to the site problem.

An alternative point of view is to regard a site as occupied if and only if it is an end-point of an occupied bond. The minimum valence of an occupied site is then unity, so that

$$\langle v_1(p)\rangle_E = \sum_{i=1}^{Q} i\binom{Q}{i}p^i q^{Q-i} \Big/ \sum_{i=1}^{Q}\binom{Q}{i}p^i q^{Q-i}$$
$$= Qp/(1-q^Q). \tag{2.2}$$

For each of these possibilities we can define the mean valence of a site in an infinite bond cluster, $\langle v_k(p)\rangle_I$, and the mean valence of a site in a finite bond cluster, $\langle v_k(p)\rangle_F$, $k = 0, 1$. For an infinite cluster, the mean valence of a site is identical for the two alternatives, while finite clusters include clusters with zero bonds in the first case but not in the second. We can write

$$\langle v_k(p)\rangle_E = P(p,k)\langle v_k(p)\rangle_I + [1-P(p,k)]\langle v_k(p)\rangle_F. \tag{2.3}$$

$P(p, 0)$ is the probability that a randomly chosen lattice site (which may have zero valence) is in an infinite bond cluster, while $P(p, 1)$ is the probability that a randomly chosen lattice site *which is the end-point of at least one occupied bond* is in an infinite bond cluster. It is easily shown that

$$P(p,0) = (1-q^Q)P(p,1). \tag{2.4}$$

Since $\langle v_0(p)\rangle_I = \langle v_1(p)\rangle_I$, we obtain

$$\langle v_0(p)\rangle_F = \langle v_1(p)\rangle_F \frac{(1-q^Q)[1-P(p,1)]}{1-(1-q^Q)P(p,1)}, \tag{2.5}$$

which implies that the leading singular behaviour of $\langle v_0(p)\rangle_F$ is the same as that of $\langle v_1(p)\rangle_F$.

In a similar way we define $f_i^X(p,k)$ to be the fraction of sites with valence i, at bond density p, given that they are members of finite ($X = F$), infinite ($X = I$) or all ($X = E$) clusters, when sites have a minimum allowed valence equal to k. Clearly

$$f_i^I(p,0) = f_i^I(p,1), \qquad i \geq 1, \tag{2.6}$$

$$f_i^E(p,0) = \binom{Q}{i}p^i q^{Q-i}, \qquad i \geq 0, \tag{2.7}$$

and

$$f_i^E(p,1) = f_i^E(p,0)/(1-q^Q), \qquad i \geq 1. \tag{2.8}$$

In the remainder of this paper we adopt the point of view that *all* lattice sites are occupied, and we write $P(p, 0) \equiv P(p)$, with a similar convention for all other properties. Corresponding quantities in the alternative convention can be obtained using the above equations.

3. Bethe approximation

The approach used in this section is to consider every point to be an *interior* point on a Bethe lattice B_Q of coordination number Q (see e.g. Essam 1972). Since surface effects are neglected, this is not an exact calculation for a Bethe lattice and, for that reason, we prefer to describe it as a Bethe approximation.

Let

$$\overline{P(p)} = 1 - P(p) \tag{3.1}$$

and

$$D(p)^Q = \overline{P(p)}. \tag{3.2}$$

$D(p)$ is conveniently calculated by noticing that it satisfies the relation (Essam 1972)

$$D(p) = q + pD(p)^\sigma \tag{3.3}$$

where $q = 1-p$ and $\sigma = Q-1$. One solution of this equation is $D(p) = 1$ (the low-density branch), and the other physically interesting solution (the high-density branch) satisfies $D(1) = 0$.

We define $P_i(p)$ to be the probability that a randomly chosen site, with valence i, is a member of an infinite bond cluster, and

$$\overline{P_i(p)} = 1 - P_i(p). \tag{3.4}$$

In order to calculate $\overline{P_i(p)}$, we note that a valence-i site is connected to i other sites by *occupied bonds*, and is not a member of an infinite cluster, if and only if *none* of these i neighbouring sites have infinite walks of occupied bonds emanating from them. Hence

$$\overline{P_i(p)} = [D(p)^\sigma]^i. \tag{3.5}$$

Let s be a lattice site, V_i be the set of sites having valence i, and I be the set of sites in infinite clusters.

$$\text{Prob}\{s \in V_i \text{ and } s \in I\} = \text{Prob}\{s \in V_i\}\text{Prob}\{s \in I | s \in V_i\} = \text{Prob}\{s \in I\}\ \text{Prob}\{s \in V_i | s \in I\}. \tag{3.6}$$

Rewriting this in the notation of the present section, we obtain

$$f_i^{\mathrm{E}}(p) P_i(p) = P(p) f_i^{\mathrm{I}}(p) \tag{3.7}$$

and hence

$$f_i^{\mathrm{I}}(p) = \frac{\binom{Q}{i} p^i (1-p)^{Q-i} [1 - D(p)^{\sigma i}]}{[1 - D(p)^Q]}. \tag{3.8}$$

In the same way

$$\text{Prob}\{s \in V_i\} = \text{Prob}\{s \in V_i | s \in I\}\ \text{Prob}\{s \in I\} + \text{Prob}\{s \in V_i | s \notin I\}(1 - \text{Prob}\{s \in I\}) \tag{3.9}$$

or

$$f_i^{\mathrm{E}}(p) = f_i^{\mathrm{I}}(p)P(p) + f_i^{\mathrm{F}}(p)(1-P(p)) \tag{3.10}$$

from which

$$f_i^{\mathrm{F}}(p) = \binom{Q}{i} p^i (1-p)^{Q-i} D(p)^{\sigma i - Q} \tag{3.11}$$

and

$$\langle v(p) \rangle_{\mathrm{F}} = pQD^{\sigma-1}. \tag{3.12}$$

Essam (1972) has pointed out that the high-density branch of $D(p)$ is regular at p_c and, extending his argument, it is straightforward to show that

$$\begin{aligned} D(p) &= 1 - \frac{2(p-p_c)}{p(\sigma-1)} - \frac{4(\sigma-2)(p-p_c)^2}{3p^2(\sigma-1)^2} + \dots \\ &= 1 - \frac{2\sigma(p-p_c)}{\sigma-1} + \frac{2\sigma^2(\sigma+1)}{3(\sigma-1)^2}(p-p_c)^2 + \dots . \end{aligned} \tag{3.13}$$

Substituting (3.13) into (3.11) gives

$$f_i^{\mathrm{F}}(p) = f_i^{\mathrm{F}}(p_c)\left(1 + \frac{\sigma}{\sigma-1}(1+\sigma-\sigma i)(p-p_c) + \mathrm{O}(p-p_c)^2\right), \qquad p \geqslant p_c. \tag{3.14}$$

For $\sigma \geqslant 2$ the linear term is positive for $i = 0, 1$ and negative for $i \geqslant 2$, so that f_0^{F} and f_1^{F} will increase just above P_c while f_2^{F}, f_3^{F} etc will decrease. Similarly, from (3.12) and (3.13)

$$\langle v(p) \rangle_{\mathrm{F}} = Qp_c - (2\sigma - Q)(p-p_c) + \mathrm{O}(p-p_c)^2. \tag{3.15}$$

In a similar way, we can investigate the p dependence of $f_i^{\mathrm{I}}(p)$, just above p_c, using (3.8) and (3.13). The result is

$$f_i^{\mathrm{I}}(p) = \frac{\sigma!(\sigma-1)^{\sigma+1-i}}{\sigma^{\sigma}(i-1)!(\sigma+1-i)!}[1 + \mathrm{O}(p-p_c)^2]. \tag{3.16}$$

The most interesting aspect of this equation is the absence of a term linear in $p - p_c$.

At the critical density, (3.16) gives

$$f_1^{\mathrm{I}}(p_c) = [(\sigma-1)/\sigma]^{\sigma}, \tag{3.17}$$

$$f_2^{\mathrm{I}}(p_c) = [(\sigma-1)/\sigma]^{\sigma-1} \tag{3.18}$$

and, in general,

$$f_{i+1}^{\mathrm{I}}(p_c)/f_i^{\mathrm{I}}(p_c) = (\sigma+1-i)/i(\sigma-1), \qquad i \geqslant 1, \tag{3.19}$$

so that, for $i > 2$, $f_i^{\mathrm{I}}(p_c)$ is a monotone decreasing function of i for any value of σ. In fact $f_i^{\mathrm{I}}(p_c)$ attains its largest value for $i = 2$.

For $Q = 4$,

$$D(p) = \tfrac{1}{2}[(4-3p)/p]^{1/2} - \tfrac{1}{2}, \qquad p \geqslant \tfrac{1}{3}, \tag{3.20}$$

(Essam 1972) and f_i^{I} can then be calculated from (3.8) and (3.20). The results are given in figure 1. f_3^{I} goes through a maximum at $p = 0.75$ while the remaining functions are

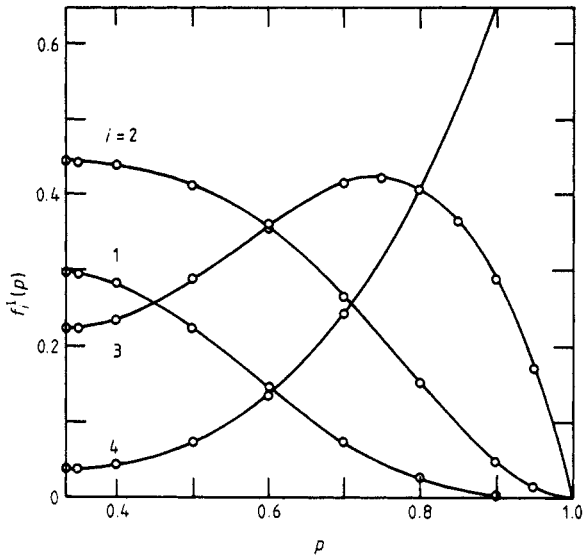

Figure 1. The p dependence of f_i^I for the $Q=4$ Bethe approximation.

monotone (cf the square lattice site percolation results of Whittington *et al* (1980)). The corresponding results for the $Q=6$ case are given in figure 2. It is interesting to note that at p_c, sites of valence less than or equal to three account for roughly 94% of the sites in infinite clusters.

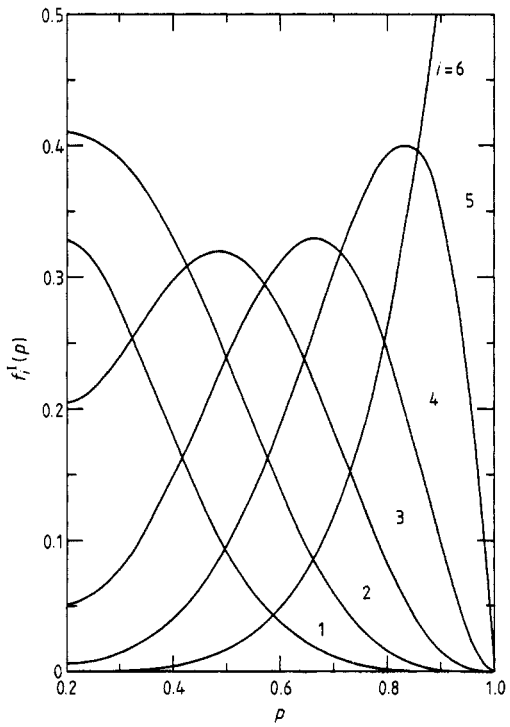

Figure 2. The p dependence of f_i^I for the $Q=6$ Bethe approximation.

The mean valence $\langle v(p)\rangle_I$ is given by

$$\langle v(p)\rangle_I = \sum_{i=1}^{Q} i f_i^I(p) = Qp(1-D(p)^{2\sigma})/(1-D(p)^Q). \tag{3.21}$$

Taking the limit $p \to p_c^+$ gives $\langle v(p_c)\rangle_I = 2$, so that the cyclomatic index of the cluster is zero (and the cluster is a tree). The mean valence increases (initially with zero slope), attaining its maximum value of Q at $p = 1$, by which time the cluster is completely compact. (Note that a calculation for a Bethe lattice *including surface effects* would give $\langle v(p)\rangle_I = 2$, $p \geqslant p_c$.)

Whittington *et al* (1980) suggested an alternative measure of the degree of ramification of a cluster based on the observation that the cyclomatic index (C) of a cluster of n sites and b bonds can be written

$$C = 1 + \tfrac{1}{2}\sum_{i=0}^{Q} (i-2)n_i \tag{3.22}$$

where n_i is the number of sites in the cluster with valence i. Since the cyclomatic index is non-negative, for an infinite cluster

$$\sum_{i=1}^{Q} (i-2) f_i^I(p) \geqslant 0 \tag{3.23}$$

and

$$\mu(p) = \sum_{i=1}^{Q} (i-2) f_i^I(p) \Big/ \sum_{i=3}^{Q} (i-2) f_i^I(p) \tag{3.24}$$

is zero if the cluster is a tree and has a maximum value of unity for a completely compact cluster.

A calculation of μ for a Bethe lattice including surface effects would give $\mu(p) = 0$ for all $p \geqslant p_c$, since all clusters are trees. Using (3.8), which was derived for the *interior* of a Bethe lattice, gives $\mu(p_c) = 0$ but μ then increases monotonically to a value of unity at $p = 1$.

4. Series derivation and analysis for finite clusters

For densities below the critical density, all clusters are finite clusters and, from (2.7),

$$f_i^F(p) = \binom{Q}{i} p^i (1-p)^{Q-i}. \tag{4.1}$$

To describe the high-density behaviour of f_i^F, we define $C(n, t, i)$ to be the number (per lattice site) of sites having valence i in clusters of n bonds ($n \geqslant 0$), with bond perimeter t. Then f_i^F is given by

$$f_i^F(q) = \sum_{n,t} C(n, t, i) q^t (1-q)^n \Big/ \sum_{n,t,i} C(n, t, i) q^t (1-q)^n \tag{4.2}$$

where $q = 1-p$. We have calculated, using an enumeration programme, $C(n, t, i)$ for $n \leqslant 12$ for the square lattice and $n \leqslant 9$ for the simple cubic lattice. Using these data

alone, the expansion of the numerators and denominator in (4.2), for the square lattice, would be correct only to order q^{13}. This would lead to expansions for f_i^F correct only to order q^9. To extend these series to order q^{11} we have included all clusters with a bond perimeter less than or equal to fifteen. In a similar way, we have included all clusters with a bond perimeter of less than or equal to thirty for the cubic lattice, and some additional data for f_5^F and f_6^F. The series for the square lattice are

$$f_0^F = 1 - 4q^2 + 4q^3 - 6q^4 + 4q^5 + 10q^6 - 48q^7 + 106q^8 - 148q^9 - 138q^{10} + 1540q^{11} + \ldots, \tag{4.3}$$

$$f_1^F = 4q^2 - 4q^3 - 4q^4 + 16q^5 - 52q^6 + 112q^7 - 188q^8 + 176q^9 + 196q^{10} - 1488q^{11} + \ldots, \tag{4.4}$$

$$f_2^F = 10q^4 - 20q^5 + 26q^6 - 16q^7 - 50q^8 + 256q^9 - 654q^{10} + 1112q^{11} + \ldots, \tag{4.5}$$

$$f_3^F = 16q^6 - 48q^7 + 116q^8 - 220q^9 + 388q^{10} - 588q^{11} + \ldots, \tag{4.6}$$

$$f_4^F = 16q^8 - 64q^9 + 208q^{10} - 576q^{11} + \ldots, \tag{4.7}$$

and, for the simple cubic lattice,

$$f_0^F = 1 - 6q^4 + 6q^5 - 9q^8 + 18q^9 - 21q^{10} + 64q^{12} - 72q^{13} - 84q^{14} + 104q^{15} + 483q^{16} - 1404q^{17} + 1418q^{18} + 768q^{19} - 4047q^{20} + 2160q^{21} + 9048q^{22} - 10\,512q^{23} - 39\,244q^{24} + \ldots, \tag{4.8}$$

$$f_1^F = 6q^4 - 6q^5 - 6q^8 + 12q^9 - 6q^{10} + 24q^{11} - 120q^{12} + 216q^{13} - 192q^{14} + 216q^{15} - 660q^{16} + 1584q^{17} - 2268q^{18} + 1140q^{19} + 1812q^{20} - 1200q^{21} - 8064q^{22} + 13\,296q^{23} + 13\,998q^{24} + \ldots, \tag{4.9}$$

$$f_2^F = 15q^8 - 30q^9 + 27q^{10} - 24q^{11} + 36q^{12} - 84q^{13} + 168q^{14} - 156q^{15} - 54q^{16} + 228q^{17} - 132q^{18} + 60q^{19} - 558q^{20} + 2436q^{21} - 6660q^{22} + 10\,008q^{23} - 1467q^{24} + \ldots, \tag{4.10}$$

$$f_3^F = 20q^{12} - 60q^{13} + 108q^{14} - 164q^{15} + 216q^{16} - 348q^{17} + 820q^{18} - 1620q^{19} + 2208q^{20} - 2484q^{21} + 3888q^{22} - 8856q^{23} + 19\,020q^{24} - \ldots, \tag{4.11}$$

$$f_4^F = 15q^{16} - 60q^{17} + 162q^{18} - 348q^{19} + 579q^{20} - 882q^{21} + 1680q^{22} - 3636q^{23} + 7044q^{24} - \ldots, \tag{4.12}$$

$$f_5^F = 6q^{20} - 30q^{21} + 108q^{22} - 300q^{23} + 648q^{24} - 1194q^{25} + \ldots, \tag{4.13}$$

$$f_6^F = q^{24} - 6q^{25} + 27q^{26} - 92q^{27} + \ldots. \tag{4.14}$$

At low density

$$\langle v(p) \rangle_F = Qp \tag{4.15}$$

and the high-density series are

$$\langle v(q) \rangle_F = 4q^2 - 4q^3 + 16q^4 - 24q^5 + 48q^6 - 64q^7 + 124q^8 - 228q^9 + 884q^{10} - 3332q^{11} + \ldots \tag{4.16}$$

for the square lattice, and

$$\langle v(q)\rangle_F = 6q^4 - 6q^5 + 24q^8 - 48q^9 + 48q^{10} - 24q^{11} + 12q^{12} - 132q^{13} + 468q^{14} - 588q^{15} - 60q^{16} + 756q^{17} + 576q^{18} - 4992q^{19} + 9666q^{20} - 7458q^{21} - 2460q^{22} - 9300q^{23} + 99\,546q^{24} + \ldots \quad (4.17)$$

for the simple cubic lattice.

We have evaluated Padé approximants (Gaunt and Guttmann 1974) to all these series and the results are presented in figures 3–6. The results for f_i^F for the square lattice are given in figure 3. The full curves are for the $Q = 4$ Bethe approximation ($p_c = \frac{1}{3}$) calculated from (2.7) at low density and (3.11) and (3.20) at high density. For the square lattice, the low-density branches ($p \leqslant p_c = \frac{1}{2}$) are again given by (2.7). These are identical to the Bethe approximation for $p \leqslant \frac{1}{3}$ and are shown as dotted curves for $\frac{1}{3} \leqslant p \leqslant \frac{1}{2}$. The Padé approximants to the high-density series are shown by broken curves with error bars indicating the estimated uncertainties. The approximants are unreliable

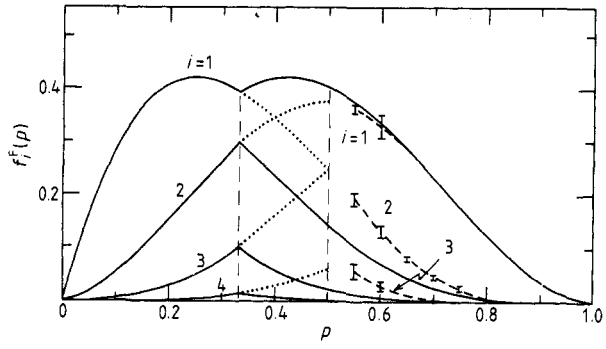

Figure 3. Comparison of the p dependence of f_i^F for the $Q = 4$ Bethe approximation (full curves) and the square lattice bond problem (broken curves above p_c, full and dotted curves below p_c, see text).

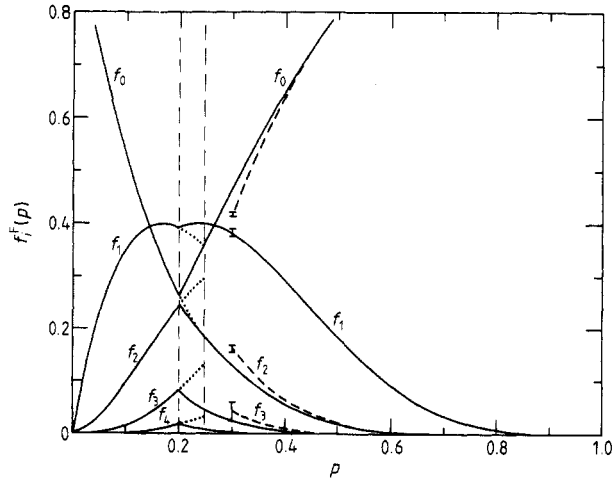

Figure 4. As figure 3, but for the $Q = 6$ Bethe approximation and the simple cubic bond problem.

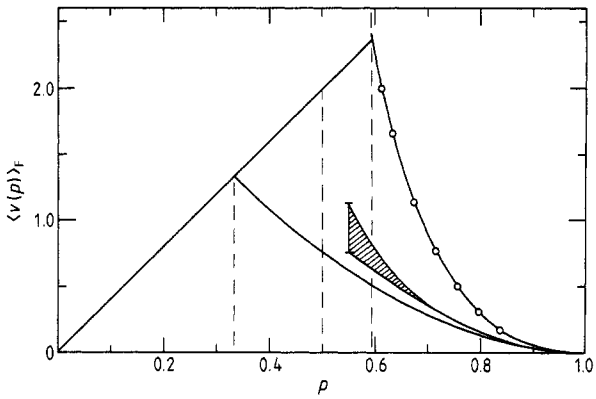

Figure 5. Comparison of $\langle v(p)\rangle_F$ for the $Q=4$ Bethe approximation (full curve), square bond (hatched) and square site (○) problems.

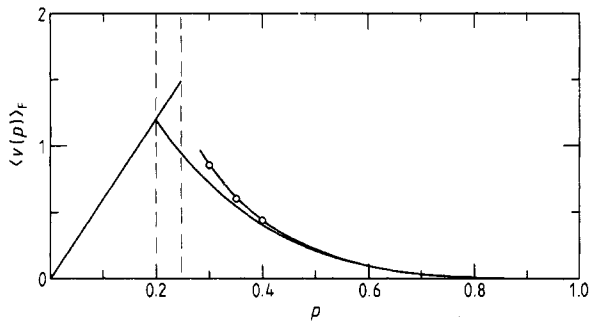

Figure 6. Comparison of $\langle v(p)\rangle_F$ for the $Q=6$ Bethe approximation (full curve) and simple cubic bond problem (○).

for $p<0{\cdot}55$ but, provided that $P(p)$ is continuous, $f_i^F(p)$ is continuous and the high- and low-density branches must match at $p_c=\frac{1}{2}$.

The corresponding results for the simple cubic lattice are shown in figure 4. The Bethe approximation to the high-density branches is much better in this case, but significant deviations still occur close to p_c. Notice that, for both lattices, the high-density branch of f_i^F must approach its value at p_c with infinite slope (Whittington *et al* 1980, (2.11) while, for the Bethe approximation, they approach linearly (equation (2.13)).

Similar remarks apply to the mean valence results shown in figures 5 and 6. The curve for the square lattice site problem is reproduced in figure 4 from Gaunt *et al* (1980) for comparison. For these finite cluster properties, the Bethe approximation is better for the bond problem than for the site problem, and better in three dimensions than in two.

5. Series derivation and analysis for infinite clusters

Properties of the infinite cluster(s) can be related to those of the finite clusters through equations such as

$$f_i^E(q)=f_i^F(q)(1-P(q))+f_i^I(q)P(q) \tag{5.1}$$

(Cherry and Domb 1980, Gaunt *et al* 1980, Whittington *et al* 1980). We have derived the series for $P(q)$ from

$$P(q) = 1 - \sum_{i \geqslant 0} \sum_{n,t} C(n, t, i) q^t (1-q)^n. \tag{5.2}$$

For the square lattice

$$\begin{aligned} P(q) = 1 &- q^4 - 4q^6 + 4q^7 - 22q^8 + 36q^9 - 118q^{10} \\ &+ 224q^{11} - 618q^{12} + 1292q^{13} - 3522q^{14} + 8564q^{15} + \ldots \end{aligned} \tag{5.3}$$

and for the simple cubic lattice

$$\begin{aligned} P(q) = 1 &- q^6 - 6q^{10} + 6q^{11} - 45q^{14} + 90q^{15} - 57q^{16} - 260q^{18} + 900q^{19} \\ &- 1200q^{20} + 572q^{21} - 1098q^{22} + 6360q^{23} - 14\,332q^{24} + 15\,444q^{25} \\ &- 12\,450q^{26} + 39\,366q^{27} - 124\,284q^{28} + 218\,028q^{29} - 256\,649q^{30} + \ldots . \end{aligned} \tag{5.4}$$

The coefficients in (5.3) have been calculated independently by J W Essam (unpublished). Combining these series with those for f_i^{F} derived in § 4 and with (2.7) yields, for the square lattice,

$$\begin{aligned} f_1^{\mathrm{I}} = {} & 4q^3 - 4q^4 - 4q^6 + 8q^7 - 16q^8 + 32q^9 - 72q^{10} + 152q^{11} \\ & - 332q^{12} + 736q^{13} - 1796q^{14} + 4584q^{15} + \ldots , \end{aligned} \tag{5.5}$$

$$\begin{aligned} f_2^{\mathrm{I}} = {} & 6q^2 - 12q^3 + 6q^4 + 6q^6 - 12q^7 + 20q^8 - 52q^9 + 144q^{10} \\ & - 380q^{11} + 962q^{12} - 2388q^{13} + 5826q^{14} - 14\,108q^{15} + \ldots , \end{aligned} \tag{5.6}$$

$$\begin{aligned} f_3^{\mathrm{I}} = {} & 4q - 12q^2 + 12q^3 - 4q^4 + 4q^5 - 12q^6 + 28q^7 - 68q^8 + 188q^9 - 500q^{10} + 1276q^{11} \\ & - 3144q^{12} + 7632q^{13} - 18\,432q^{14} + 45\,288q^{15} + \ldots , \end{aligned} \tag{5.7}$$

$$\begin{aligned} f_4^{\mathrm{I}} = {} & 1 - 4q + 6q^2 - 4q^3 + 2q^4 - 4q^5 + 10q^6 - 24q^7 + 64q^8 - 168q^9 + 428q^{10} - 1048q^{11} \\ & + 2514q^{12} - 5980q^{13} + 14\,402q^{14} - 35\,764q^{15} + \ldots . \end{aligned} \tag{5.8}$$

The corresponding series for the simple cubic lattice are

$$\begin{aligned} f_1^{\mathrm{I}} = {} & 6q^5 - 6q^6 - 6q^{10} + 12q^{11} - 6q^{12} - 30q^{14} + 96q^{15} - 108q^{16} + 24q^{17} - 120q^{18} \\ & + 756q^{19} - 1458q^{20} + 1032q^{21} - 324q^{22} + 3900q^{23} - 13\,722q^{24} \\ & + 19\,932q^{25} - 12\,120q^{26} + 15\,144q^{27} - 87\,684q^{28} + 224\,976q^{29} \\ & - 29\,2290q^{30} + \ldots , \end{aligned} \tag{5.9}$$

$$\begin{aligned} f_2^{\mathrm{I}} = {} & 15q^4 - 30q^5 + 15q^6 + 15q^{10} - 30q^{11} + 15q^{12} + 75q^{14} - 240q^{15} + 258q^{16} - 96q^{17} \\ & + 564q^{18} - 2346q^{19} + 3885q^{20} - 3108q^{21} + 4302q^{22} - 18\,294q^{23} \\ & + 44\,439q^{24} - 57\,912q^{25} + 53\,460q^{26} - 11\,9652q^{27} + 378\,270q^{28} \\ & - 740\,736q^{29} + 920\,259q^{30} - \ldots , \end{aligned} \tag{5.10}$$

$$f_3^{\mathrm{I}} = 20q^3 - 60q^4 + 60q^5 - 20q^6 + 20q^9 - 60q^{10} + 60q^{11} - 20q^{12} + 120q^{13} - 480q^{14} + 740q^{15} - 540q^{16} + 1080q^{17} - 4540q^{18} + 9540q^{19} - 10\,788q^{20} + 12\,044q^{21} - 36\,096q^{22} + 97\,248q^{23} - 157\,108q^{24} + 175\,632q^{25} - 284\,976q^{26} + 793\,512q^{27} - 1731\,612q^{28} + 2565\,444q^{29} - 3365\,400q^{30} + \ldots, \tag{5.11}$$

$$f_4^{\mathrm{I}} = 15q^2 - 60q^3 + 90q^4 - 60q^5 + 15q^6 + 15q^8 - 60q^9 + 90q^{10} - 60q^{11} + 105q^{12} - 450q^{13} + 915q^{14} - 960q^{15} + 1215q^{16} - 4200q^{17} + 10\,500q^{18} - 15\,120q^{19} + 16\,920q^{20} - 35\,730q^{21} + 99\,120q^{22} - 188\,700q^{23} + 245\,523q^{24} - 338\,502q^{25} + 796\,176q^{26} - 1867\,548q^{27} + 3168\,708q^{28} - 4346\,874q^{29} + 7346\,142q^{30} - \ldots, \tag{5.12}$$

$$f_5^{\mathrm{I}} = 6q - 30q^2 + 60q^3 - 60q^4 + 30q^5 - 6q^6 + 6q^7 - 30q^8 + 60q^9 - 60q^{10} + 66q^{11} - 222q^{12} + 546q^{13} - 750q^{14} + 870q^{15} - 2166q^{16} + 5880q^{17} - 10\,248q^{18} + 12\,816q^{19} - 21\,060q^{20} + 53\,946q^{21} - 115\,158q^{22} + 173\,778q^{23} - 233\,814q^{24} + 454\,278q^{25} - 1066\,296q^{26} + 2016\,276q^{27} - 3010\,254q^{28} + 4685\,586q^{29} - 9645\,774q^{30} + 20\,578\,704q^{31} - \ldots, \tag{5.13}$$

$$f_6^{\mathrm{I}} = 1 - 6q + 15q^2 - 20q^3 + 15q^4 - 6q^5 + 2q^6 - 6q^7 + 15q^8 - 20q^9 + 21q^{10} - 48q^{11} + 128q^{12} - 216q^{13} + 270q^{14} - 506q^{15} + 1341q^{16} - 2688q^{17} + 3844q^{18} - 5646q^{19} + 12\,501q^{20} - 28\,184q^{21} + 48\,156q^{22} - 67\,932q^{23} + 114\,682q^{24} - 253\,428q^{25} + 513\,756q^{26} - 837\,732q^{27} + 1282\,572q^{28} - 2388\,396q^{29} + 5037\,063q^{30} - \ldots. \tag{5.14}$$

Combining these gives the series for $\langle v(q)\rangle_{\mathrm{I}}$ and $\mu(q)$. For the square lattice

$$\langle v(q)\rangle_{\mathrm{I}} = 4 - 4q + 4q^4 - 4q^5 + 12q^6 - 28q^7 + 76q^8 - 180q^9 + 428q^{10} - 972q^{11} + 2216q^{12} - 5064q^{13} + 12\,168q^{14} - 30\,824q^{15} + \ldots \tag{5.15}$$

and

$$\mu(q) = 1 - 2q^3 - 2q^4 - 4q^5 - 2q^6 - 4q^7 + 4q^8 + 24q^{10} + 16q^{11} + 70q^{12} + 56q^{13} + 222q^{14} - 152q^{15} + \ldots. \tag{5.16}$$

For the simple cubic lattice

$$\langle v(q)\rangle_{\mathrm{I}} = 6 - 6q + 6q^6 - 6q^7 + 30q^{10} - 66q^{11} + 42q^{12} - 6q^{13} + 210q^{14} - 690q^{15} + 864q^{16} - 456q^{17} + 1212q^{18} - 5592q^{19} + 11\,334q^{20} - 11\,346q^{21} + 9618q^{22} - 34\,446q^{23} + 104\,946q^{24} - 172\,182q^{25} + 175\,632q^{26} - 258\,828q^{27} + 793\,014q^{28} - 1850\,106q^{29} + 2830\,104q^{30} \ldots \tag{5.17}$$

and

$$\mu(q) = 1 - 1\tfrac{1}{2}q^5 - \tfrac{3}{4}q^6 - 1\tfrac{1}{8}q^7 - 1\tfrac{11}{16}q^8 - 2\tfrac{17}{32}q^9 - \tfrac{3}{64}q^{10} - 1\tfrac{121}{128}q^{11} - \ldots \quad (5.18)$$

where we omit the higher-order terms since the fractions become awkward.

We have formed Padé approximants to each of these series. The convergence is remarkably good, and much better than for the corresponding series for finite clusters. For the square lattice bond problem the estimated p dependence of $f_i^{\mathrm{I}}(p)$ is essentially superimposable on the $Q=4$ Bethe results (figure 1) for $p > p_c = \frac{1}{2}$. The largest deviations occur at p_c, and in table 1 we compare the estimates with the Bethe approximation at $p = \frac{1}{2}$. Estimates of $f_i^{\mathrm{I}}(p)$ for the square lattice site problem have been reported elsewhere (Whittington *et al* 1980). These are also very close to the Bethe results, and the largest deviations again occur at the critical point, $p_c \simeq 0.593$. In table 1 we also give the estimates of f_i^{I} at $p = 0.6$ for the square lattice site and bond problems and for the $Q = 4$ Bethe approximation for comparison.

Table 1. Comparison of f_i^{I} for four-coordinated lattices.

	$p = 0.5$		$p = 0.6$		
	Square bond	B_4	Square site	Square bond	B_4
f_1^{I}	0.215	0.224	0.126	0.144	0.145
f_2^{I}	0.410	0.414	0.354	0.357	0.358
f_3^{I}	0.297	0.289	0.375	0.362	0.361
f_4^{I}	0.078	0.073	0.143	0.136	0.136

The $Q = 6$ Bethe results for f_i^{I} are again an excellent approximation to the bond problem on the simple cubic lattice. For $p > 0.3$ the Bethe approximation within the small uncertainties in the Padé approximants. For $i = 1$ and 2 the simple cubic curves for $p < 0.3$ deviate negatively by about 0.008 and 0.003, respectively, while for $i = 3$ and 4 the deviations are positive and about equal to 0.005 and 0.004 respectively. These deviations are in the same directions as for the square lattice (see table 1). Deviations for $i = 5$ and 6 are negligible even at p_c.

The disadvantage with this comparison is that, for instance, it compares an incipiently percolating cluster on a lattice, with infinite clusters in the corresponding Bethe approximation at a density well above the critical density. An alternative view is to take account of the differences in critical densities by using the reduced density variable

$$\rho = (p - p_c)/(1 - p_c). \quad (5.19)$$

The dependences of $\langle v(p)\rangle_{\mathrm{I}}$ and $\mu(p)$ on this reduced density are shown in figures 7–10. For the square lattice the deviations from the Bethe approximation are quite marked, and are greater for the site problem than for the bond problem. For the simple cubic lattice the deviations are much less, though this reflects, in part, the smaller difference between the critical density of the lattice and that in the corresponding Bethe approximation.

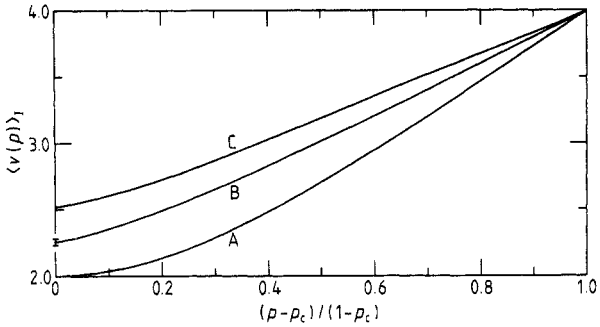

Figure 7. Comparison of $\langle v(p)\rangle_I$ for the $Q = 4$ Bethe approximation (A), square lattice bond (B) and site (C) problems.

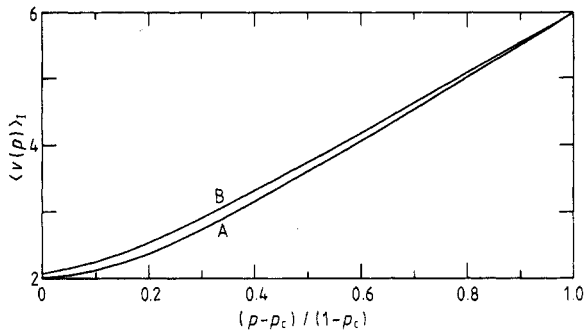

Figure 8. Comparison of $\langle v(p)\rangle_I$ for the $Q = 6$ Bethe approximation (A) and simple cubic bond problem (B).

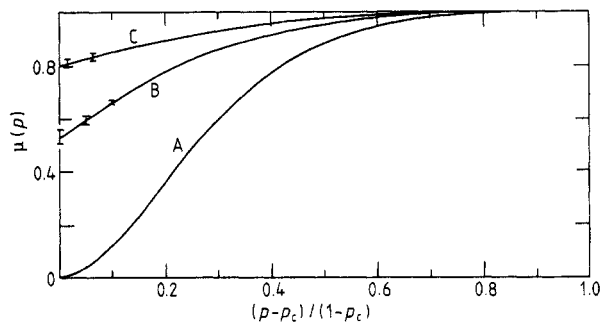

Figure 9. Comparison of $\mu(p)$ for the $Q = 4$ Bethe approximation (A), square lattice bond (B) and site (C) problems.

6. Discussion

If we write

$$\langle v(p_c^+)\rangle_F - \langle v(p)\rangle_F \sim B'(p-p_c)^{\beta'}, \qquad p \to p_c^+, \tag{6.1}$$

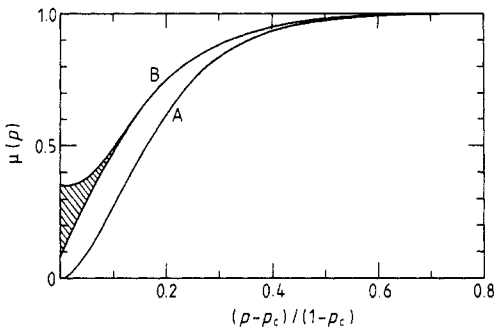

Figure 10. Comparison of $\mu(p)$ for the $Q = 6$ Bethe approximation (A) and simple cubic bond problem (B).

then Gaunt *et al* (1980) showed that, provided $P(p)$ is continuous, $\langle v(p)\rangle_F$ is continuous at p_c and $\beta' = \beta$, the exponent characterising the behaviour of $P(p)$. Our calculation for the Bethe approximation confirms this explicitly with $\beta' = \beta = 1$. $f_i^F(p)$, in the Bethe approximation, also approaches its critical value linearly, as expected from the general arguments given in Whittington *et al* (1980), and we can obtain from (3.5) and (3.13) an explicit expression for $P_i(p)$ in this approximation,

$$P_i(p) = 1 - D^{\sigma i} = \begin{cases} 0, & p \leqslant p_c, \\ 2i[\sigma^2/(\sigma-1)](p-p_c) + O(p-p_c)^2, & p \geqslant p_c, \end{cases} \tag{6.2}$$

so that, as expected (Whittington *et al* 1980), $P_i(p)$ is singular at p_c for all i, at least in this approximation. Moreover, for $Q = 4$ it is clear from (3.5) and (3.20) that $P_i(p)$ has no other singularities on the real interval (0, 1).

The Bethe approximation result (3.16) for f_i^I shows that the critical values are approached quadratically.

The series results for f_i^F shows rather poor convergence, but there is at least qualitative agreement between the behaviour for the square site and square bond problems. In the same way, the behaviour of $\langle v(p)\rangle_F$ for both the square and simple cubic lattices is similar for the site and bond versions of these problems.

The convergence for the infinite cluster data is much better than for the finite clusters and is in remarkably close agreement with the Bethe approximation. If, however, the results are considered in terms of the reduced density, ρ (equation (5.19)), it is clear that at and just above the critical density the infinite cluster is more ramified in three dimensions than in two, and more ramified for the bond problem than for the site problem. For instance, the values of $\mu(p_c)$ are zero for the Bethe approximation, about 0.2 for the simple cubic bond problem, about 0.55 for the square bond problem and about 0.8 for the square site problem.

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