THEORY OF PERCOLATION PROCESSES

by

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Abstract

Series estimates of the critical percolation probabilities and of the critical indices for the 'site problem' and the 'bond problem' are presented for two and three dimensional lattices. These critical values are also calculated exactly on the Bethe lattice. The results derived differ slightly from any previous values, and are consistent with the assumption of a constant gap index Δ in both two and three dimensions. The relation between the critical indices $\gamma = (3-g)\Delta$ is deduced and shown to hold on the Bethe lattice. The series estimates are also consistent with the above result.

An analogy is drawn between the mean number of clusters and the free energy of a ferromagnet. The corresponding scaling laws, describing the behaviour near the critical point, are tested using the exact solution for the Bethe lattice. Numerical work on the moments of the cluster size distribution for two and three dimensional lattices is found to be consistent with the scaling hypothesis. The strong or weak k weight of a graph is shown to have the property $\sum_{G' \subseteq G} k(G')v(G') = n(G) - B$.

The critical index δ , which describes the variation of the magnetisation with the field near the critical point, $(M \sim H^{1/\delta})$ is calculated and shown to have different values at two points on the phase boundary.

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Chapter 1 Introduction

1.1 General Discussion of Percolation Systems

The percolation model was first introduced by Broadbent and Hammersley [1] to describe, for example, the behaviour of a fluid seeping into a porous solid or the spread of disease in an orchard. In the case of the porous solid they considered the 'pores' or channels of the solid to be open or closed in a random manner. If the channel was open the fluid could pass along it otherwise it could not. The problem was to calculate the minimum concentration of open channels which were required before the fluid could 'percolate' throughout the solid. For the orchard problem the trees were considered to be diseased or free of disease in a random manner. The problem was to determine the minimum concentration of diseased trees necessary for an epidemic to occur.

The above problems are formulated theoretically in the following manner. The solid is considered to be a random medium[1] consisting of an infinite number of sites connected by bonds. We may consider either the sites or the bonds to be occupied independently with probability p or unoccupied independently with probability $q = 1-p$. The two problems have become known as the site problem and the bond problem respectively.

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(1) A random medium is a medium in which the sites (bonds) are occupied independently.

The flow of fluid in a porous solid is an example of the bond problem. Here the occupied bonds are the open channels and the unoccupied bonds the closed channels. The fluid flows along the occupied bonds and 'wets' each site it passes. If the fluid is to wet an infinite number of sites then a certain concentration of the bonds must be occupied. For p less than this critical value p_c the fluid can only form isolated 'pockets' or clusters in the medium. A cluster is defined such that there is an occupied path of bonds between any two sites belonging to the same cluster.

The spread of disease in an orchard is a site problem. Here the occupied sites are the diseased trees and the unoccupied sites the trees free of disease. For an epidemic to occur a certain concentration of occupied sites, i.e. diseased trees, is required. For p less than this critical value p_c the disease is localised and does not spread throughout the orchard.

We define p_c more exactly in terms of the percolation probability $P(p)$, which is the probability that a given site belongs to a cluster of infinite size. Therefore by definition $P(p) = 0$ for $p < p_c$, and p_c is defined such that

$$p_c = \sup\{p, \text{ such that } P(p)=0\} \quad . \tag{1.10}$$

There are few exact relations concerning the percolation probability $P(p)$ but Hammersley [2] has shown that

$$P_N^s(p) \leq P_N^b(p) \tag{1.11}$$

where s and b denote the site and bond problems respectively and $P_N(p)$ is the probability that any given site belongs to a cluster of size N . From (1.11) we obtain

$$P^s(p) \leq P^b(p) \tag{1.12}$$

since $P(p) = \lim_{N\to\infty} P_N(p)$.

So that if $P(p)$ is a monotonic increasing function of p then

$$p_c^s \leq p_c^b \quad . \tag{1.13}$$

It is possible to calculate $P(p)$ exactly (see chapter 4) on lattices with a tree like structure, i.e. they contain no loops. We obtain

$$P(p) \sim (p-p_c)^{\Delta-\gamma} \tag{1.14}$$

for $p \to p_c^+$. (The critical indices Δ and γ are explained in section 1.2.)

To obtain inequalities for the critical concentration p_c we consider the number of n-stepped self-avoiding walks on a random medium. (An n-stepped self-avoiding walk is an ordered continuous sequence of n steps, along the edges, from site to site and which visits no site more than once.) We define the connective constant μ as

$$\ln \mu = \lim_{n\to\infty} \frac{1}{n} \ln C_n \quad . \tag{1.15}$$

Broadbent and Hammersley show in [1] that a rigorous lower bound on p_c is provided by

$$p_c \geq \frac{1}{\mu} \quad . \tag{1.16}$$

This holds for both site and bond problems.

Several other rigorous bounds and inequalities have been obtained for p_c on specific lattices by introducing associated lattices. Using these properties exact values of p_c, on certain two dimensional lattices, have been obtained.

a) For the bond problem we associate with any planar lattice L a <u>dual lattice</u> L^D. The dual lattice is defined such that each bond of L^D intersects a bond of the original lattice once and once only, and vice versa (see Fig. 1.1).

Essam [3] has shown that for a lattice and its dual

$$p_c(b,L) + p_c(b,L^D) = 1 \tag{1.17}$$

where $p_c(b,L)$ and $p_c(b,L^D)$ are the critical concentrations on L and L^D respectively.

Since the square lattice is its own dual it immediately follows that $p_c(b,S) = \frac{1}{2}$. The dual of the triangular lattice is the honeycomb lattice and Sykes and Essam [20] have shown using a star triangle transformation that

$$p_c(b,T) = 2\sin(\pi/18)$$

$$p_c(b,H) = 1 - 2\sin(\pi/18) \quad .$$

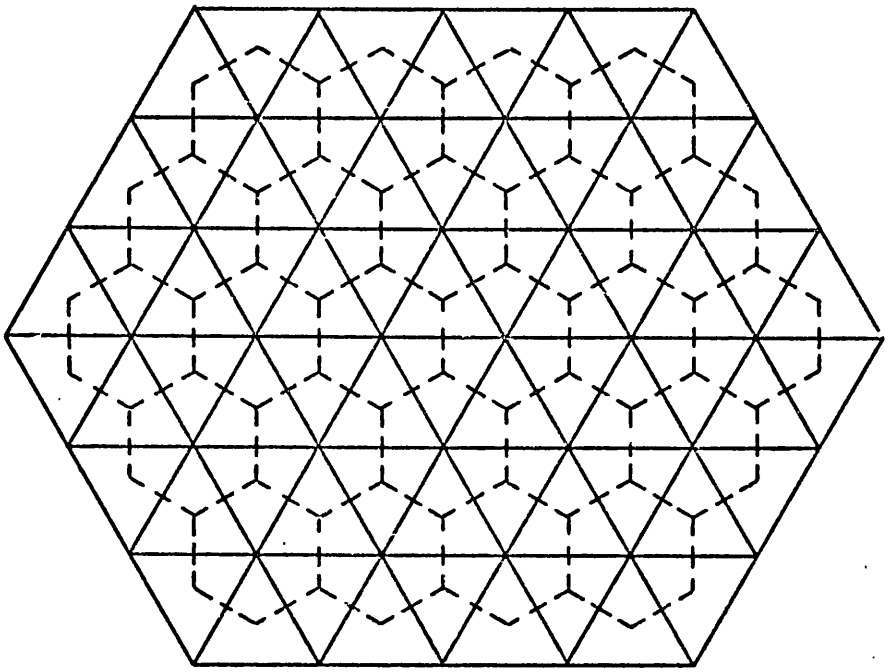
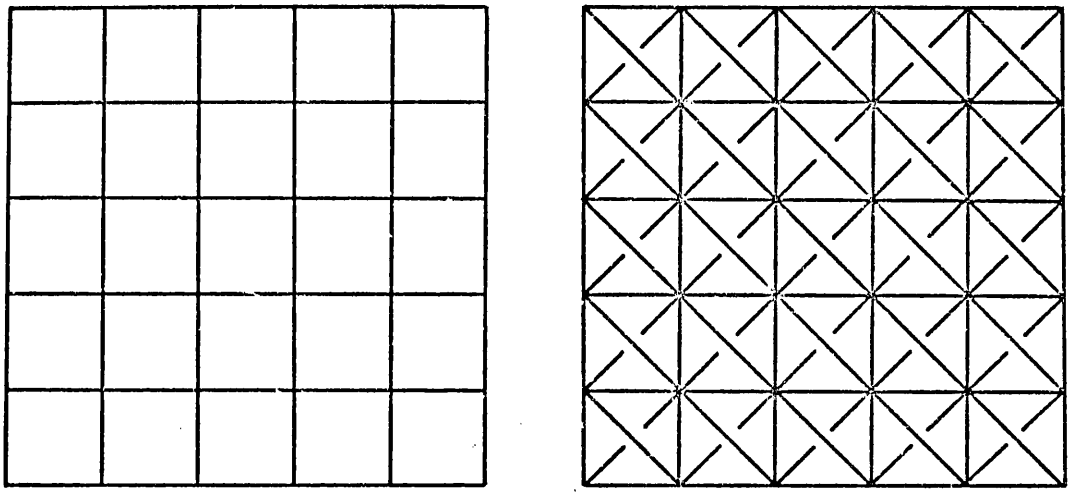


Fig. 1.1 The triangular lattice and its dual the honeycomb showing the basic property of the intersection of the lattices.

b) For the site problem we associate with any two dimensional lattice L a matching lattice L* (see appendix V). In Fig. 1.2 we show the square lattice and its matching lattice. Sykes and Essam [20] have shown that the critical concentrations of the two lattices are complimentary, i.e.

$$p_c(s,L) + p_c(s,L^*) = 1 \quad . \tag{1.18}$$

Since the triangular lattice is its own matching lattice it follows that $p_c(s,T) = \frac{1}{2}$.

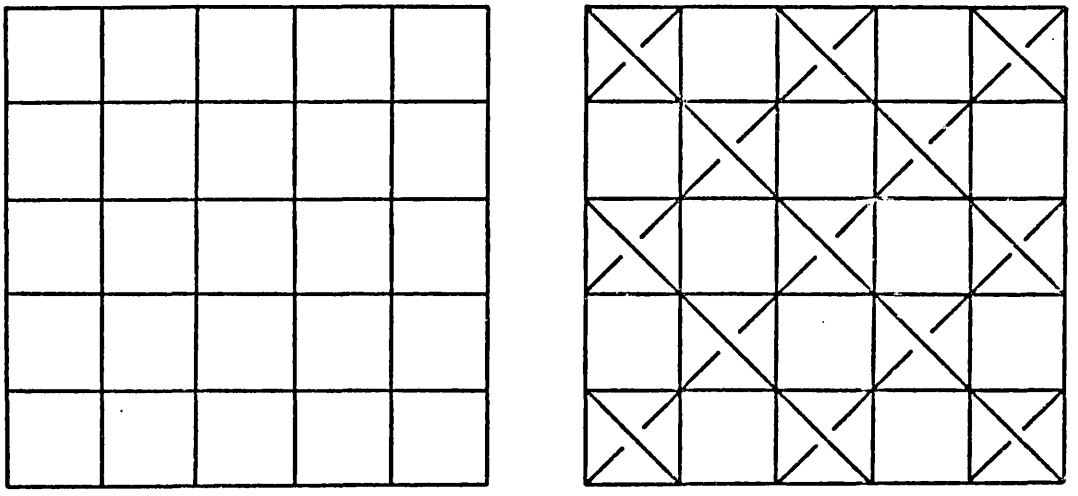


(A) (B)

Fig. 1.2 (A) The square lattice (B) The corresponding matching lattice.

c) We consider now the relation between the site and the bond problems. A bond problem on any lattice L is isomorphic with the site problem on a suitably defined covering lattice L^c. (See Fig. 1.3). (For a definition of the covering lattice see appendix V). Any configuration of occupied bonds on any lattice is in one to one correspondence with the occupied sites on the covering lattice, therefore the characteristic properties of the bond problem on L are identical with those of the site problem on L^c. Particularly

$$p_c(b,L) = p_c(s,L^c) \quad . \tag{1.19}$$



(A) (B)

Fig. 1.3 (A) The square lattice (B) The covering lattice of the square lattice, S^c .

It is interesting to note that $p_c(s,S^c)$ is a self matching lattice and therefore $p_c(s,S^c) = \frac{1}{2}$, a value already derived from the self-duality of the square lattice. The covering lattice of the honeycomb is the kagomé lattice, while that of the triangular is the kagomé matching lattice. Both $p_c(b,H)$ and $p_c(b,T)$ are known therefore we also know $p_c(s,K)$ and $p_c(s,K^*)$. Since to every bond problem one can associate an equivalent site problem while the converse is not true, the site problem is of greater generality.

One of the best known examples of the site problem is that of the dilute ferromagnet. Here the occupied sites are magnetic atoms

and the unoccupied sites non-magnetic impurities. Below the critical concentration p_c no spontaneous magnetisation occurs at any temperature since the magnetic atoms can only form finite isolated clusters. Above p_c the spontaneous magnetisation occurs at a critical temperature $T_c(p)$ which falls to zero at $p = p_c$. (See Fig. 1.4.)

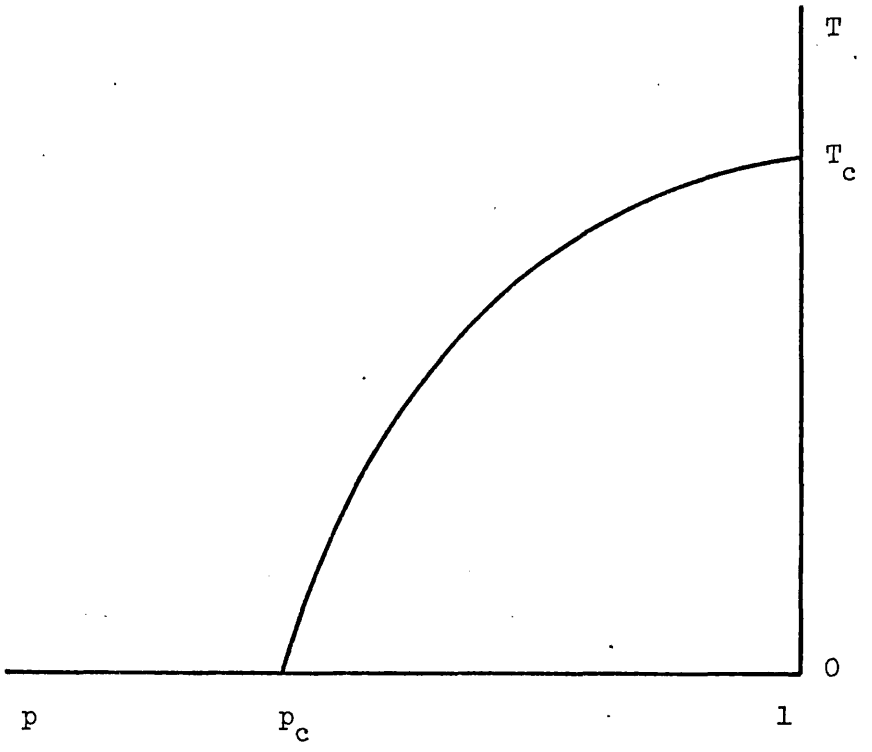


Fig. 1.4 Diagramatic representation of the variation of the critical temperature $T_c(p)$ with p .

If the interactions between the magnetic atoms are assumed to be Ising like then Fortuin and Kasteleyn [30] have shown, using the random cluster model, that the mean number of clusters per site is related to the free energy, $P(p)$ is related to the spontaneous magnetisation while the mean size of clusters per site

is the susceptibility analogue.

Dalton, Domb and Sykes [4] have shown for the site problem that for lattices with a large coordination number Z, $p_c Z$ tends to a limiting value A. Where the constant A depends only on the dimensionality of the lattice and is independant of any special lattice structure. In two dimensions A was found to be approximately 4.5 while in three dimensions A was approximately 2.7. We can interpret these values as being the number of occupied points, for a given dimensionality, which have to be within range of a given point for an infinite cluster to exist. The independence of A on any special lattice structure can be seen more clearly in the case of random or continuous percolation. An example of such a problem in two dimensions is that of the relay stations [5]. Here the question is how many stations per unit area are required to provide long range communication when the stations are distributed at random and can communicate directly if the distance between them is less than a distance R. We associate this with a percolation system in the following manner. If we have a lattice of coordination number Z then the mean number of sites adjacent to a given site is Zp. In the random case the value is $V_d(R)D$. Where $V_d(R)$ is the volume of a d-dimensional sphere and D is the density of distribution of the sites.

We use the independence of A on the lattice structure to obtain estimates for D_c. In the limiting case

$$p_c = \frac{V_d(R)D_c}{Z} \quad . \qquad (1.20)$$

From above, in two dimensions

$$4.5 = \pi R^2 D_c$$

$$= 4\pi t_{2c} \qquad \text{where} \qquad t_{2c} = D_c \left(\frac{R}{2}\right)^2$$

hence

$$t_{2c} = 0.36 \quad .$$

In three dimensions

$$2.7 = 4/3\ \pi R^3 D_c$$

$$2.7 = \frac{32\pi}{3}\ t_{3c}$$

$$t_{3c} = 0.081 \quad .$$

Roberts and Storey [35],[36] obtain direct estimates of t_{2c} and t_{3c} using Monte Carlo techniques and they obtain the values of $t_{2c} = 0.304$ and $t_{3c} = 0.0889$. These two results indicate clearly the independence of A on the lattice structure. Although no exact values are known for t_{2c} we may use exact results derived on a two dimensional lattice structure to provide an upper bound for the critical concentration. (See chapter 3.)

1.2 Graph Theory Terminology: Mean Values and Perimeter Distribution

The percolation problem is discussed in graph theoretical concepts and we shall develop those needed below. The discussion will be in terms of finite graphs which will be extended to cover

the infinite case at a later stage.

Consider a general linear graph $G = (V,E)$ with vertex set V and edge set E. In the site problem the vertices of the graph are the possible locations of a particle and an edge $[i,j] \in E$ is said to be occupied if both its vertices are occupied by a particle. The edges are usually the nearest neighbour pairs of sites though higher order neighbours may be included. The subset $V' \subseteq V$ consisting of all occupied vertices defines a section graph $G' = (V',E')$ where E' consists of all the edges of E with both vertices in V'. Each component of G' corresponds to a cluster of particles in this configuration. We define the expectation value of a function of the state of the system

$$\langle A;G \rangle = \sum_{V' \subseteq V} \pi(V')A(V',G) \qquad (1.21)$$

where the sum runs over all section graphs of G and $\pi(V')$ is the probability that the vertices V' are occupied and the vertices $V-V'$ are unoccupied.

There are $2^{|V|}$ terms in the sum and $\pi(V')$ is normalised to one.

Because we shall consider only those systems where the sites are occupied independently, i.e. a random medium

$$\pi(V') = p^{|V'|}q^{|V-V'|} \quad . \qquad (1.22)$$

In the case of the bond problem it is the edges of the graph which are in one of the two states and the occupied edges define a <u>partial graph</u> $G' = (V,E')$. Note there is no restriction on the edge set $E' \subseteq E$ and G' contains the complete vertex set. Definition (1.21) becomes

$$\langle A;G\rangle = \sum_{E' \subseteq E} \overline{\pi}(E')A(E',G) \tag{1.23}$$

where the sum runs over all partial graphs and

$$\overline{\pi}(E') = p^{|E'|}q^{|E-E'|} \quad . \tag{1.24}$$

If we are going to use (1.21) to obtain mean values then it is necessary to sum over all the $2^{|V|}$ configurations. For a large graph this becomes difficult and Domb has shown [8] that it is only necessary to sum over those configurations which are connected. The probability that a connected set Γ of s vertices occurs as a cluster is $p^s q^w$, where w is the number of vertices not in Γ but adjacent to vertices in Γ and is known as the perimeter of Γ . Similarly we may define a bond perimeter where w is now the number of edges not contained in Γ but connected to vertices in Γ .

Using the above restricted class of graphs and assuming $A(V',G)$ is additive (1.21) becomes

$$\langle A;G\rangle = \sum_{V' \subseteq V} \pi^*(V')A(V',G) \tag{1.25}$$

where now the sum runs only over all connected section graphs of G and

$$\pi^*(V') = p^{|V'|} q^w$$

where w is the perimeter of $G' = (V', E')$.

We now introduce an important concept in percolation theory, that of the perimeter distribution over a set of graphs of a given size. We can write (1.25) in the form

$$\langle A;G \rangle = \sum_{s,w} b_{s,w} p^s q^w$$

where $b_{s,w}$ is the weighted sum of connected section graphs of G with s vertices, the corresponding clusters of which have perimeter w. The weighting of $b_{s,w}$ depends on the particular mean value being calculated. For example if the mean size is being calculated where each connected graph is weighted with the product of its vertices and edges

$$b_{s,w} = s \sum_{\substack{V' \subset V \\ |V'|=s}} e$$

where $e = |E'|$ and the sum runs only over those graphs with perimeter w.

It is necessary to sum over both s and w since different configurations of s vertices may have different perimeters. (See Fig. 1.5.) It is this fact, together with the way in which $a_{s,w}$ varies for large s, which provides one of the major difficulties

in deriving exact relations for cluster expansions on an infinite lattice. It is thought that the average perimeter varies directly with the size of the graph as $s \to \infty$ (s is the number of sites (edges) the graph contains) though this has not been rigorously proved. We can place bounds on the perimeter distribution in the following way. The minimum perimeter is obtained when the sites are as closely packed as possible and a geometrical representation of this is the d-dimensional hypersphere. If we associate one site per unit volume then the perimeter is represented by the surface of the hypersphere. Hence we see that the perimeter in d dimensions must vary at least like $s^{d-1/d}$. It is easy to see that the perimeter can vary at most like s since the maximum perimeter of a graph of s sites on a lattice of coordination number Z is $Zs - 2(s-1)$. Therefore we can write

$$s^{d-1/d} < w \leq s \tag{1.27}$$

where this is taken to mean w varies asymtotically at least like $s^{d-1/d}$ and at most like s.

As $d \to \infty$ the two limits approach and for a lattice of infinite dimension w must vary like s. We can see this in the case of the Bethe lattice (see Fig. 1.6) which is an infinite tree every vertex being of degree $Z = \sigma + 1$.

Here there is an exact relation between the size and the perimeter and between the lattice count and the size and this has enabled the lattice to be solved exactly. (See chapters 2 and 4.)

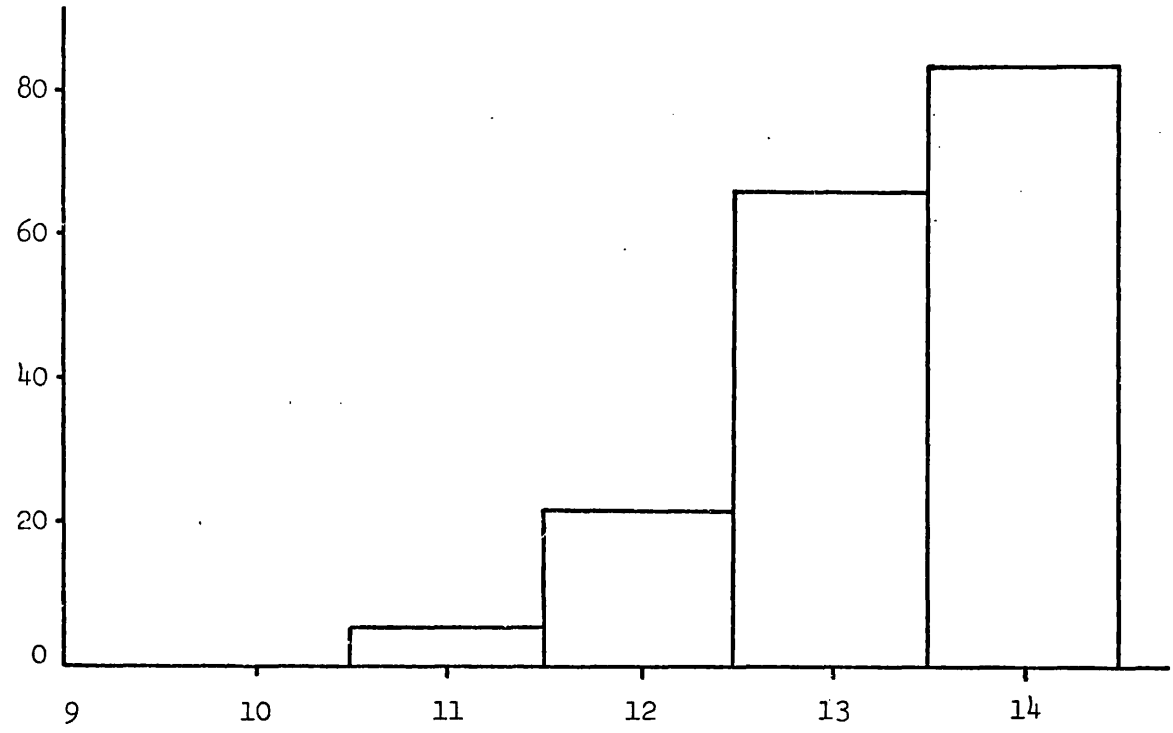


Fig. 1.5 Distribution of the perimeter for size $s = 5$ on the triangular lattice site problem.

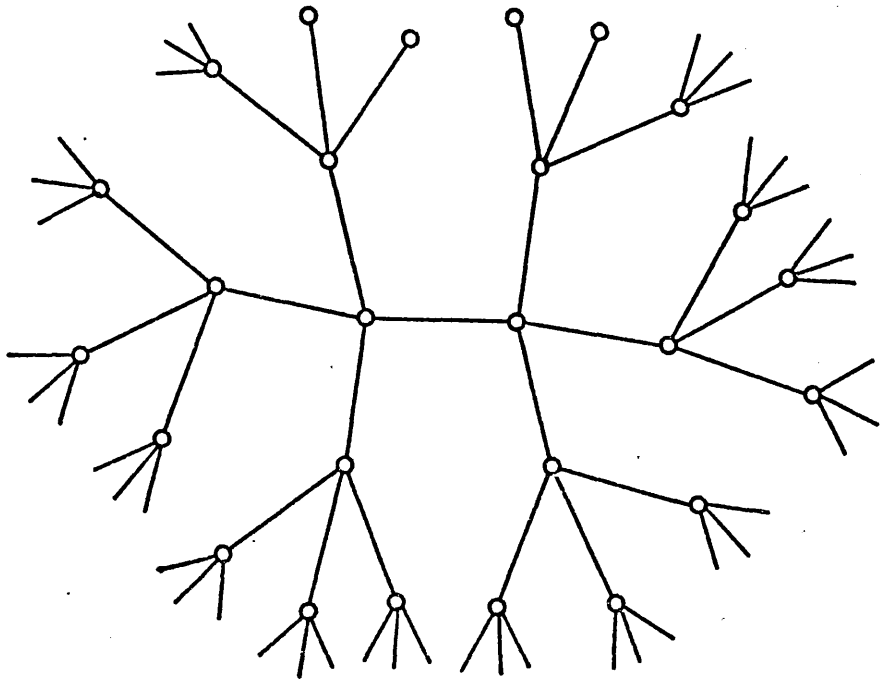


Fig. 1.6 Bethe lattice of coordination number four.

We have tried to approach the problem through a numerical treatment. If we define the average perimeter for a given size s as

$$\bar{w}_s = \frac{\sum_w a_{s,w} w}{\sum_w a_{s,w}} \tag{1.28}$$

where $a_{s,w}$ is the number of connected section graphs per site of the lattice of size s and perimeter w.

If the average perimeter varies as s then

$$\bar{w}_s \underset{s\to\infty}{\sim} s \quad .$$

If we write $\bar{w}_s = cs + d$ then

$$\frac{\bar{w}_s}{\bar{w}_{s-1}} = \nu_s = 1 + \frac{1}{s} + \left(1 - \frac{d}{c}\right)\frac{1}{s^2} \quad .$$

To test this relation we have fitted the ν_s to a curve of the form $1 + \frac{A}{s} + \frac{B}{s^2}$. If the perimeter varies directly with s then we should obtain a value of one for A and the intercept of ν_s plotted against $\frac{1}{s}$ should be one. On all the lattices considered (the data is recorded in appendix VI) the final value of A was very close to one. In all cases it was greater than 0.92 and appeared to be steadily increasing to one. The intercept on the ν_s axis also appeared to converge to the value one. We conclude that the evidence is not inconsistent with the assumption that $\bar{w}_s \underset{s\to\infty}{\sim} s$ but larger cluster expansions should provide more

conclusive results.

We have so far defined in a general way the mean value of any function of state of the system. We shall be particularly concerned here with the moment distributions of the cluster size. The zeroeth moment or the mean number of clusters is defined as

$$k(p,L) = \sum_s \langle n_s(p) \rangle \tag{1.29}$$

where $\langle n_s(p) \rangle$ is the mean number of clusters, of size s, per site.

$$\langle n_s(p) \rangle = \sum_w a_{s,w} p^s q^w$$

(In Figs. 1.7 and 1.8 $\langle n_s(p) \rangle$ for the Bethe lattice is plotted as a function of p and as a function of s.)

Only one exact result (other than on the Bethe lattice) is known concerning $k(p,L)$. Temperley and Lieb have shown [37] that for $p = p_c = \frac{1}{2}$ on the square lattice (bond problem).

$$k(p_c,L) = \left| \frac{1}{2} \frac{\partial}{\partial z} \exp\left\{ \frac{1}{4\mu} \int_{-\infty}^{\infty} d\alpha \operatorname{sech}\left(\frac{\pi\alpha}{2\mu}\right) \ln\left(\frac{\cosh\alpha - \cos 2\mu}{\cosh\alpha - 1}\right) \right\} \right|_{z=1}$$

$$\simeq 0.0981 \tag{1.30}$$

where $\cos\mu = \frac{z}{2}$.

We show in chapter 4 that for large s

$$\langle n_s(p) \rangle \sim \mu(p)^s s^{-g} \tag{1.31}$$

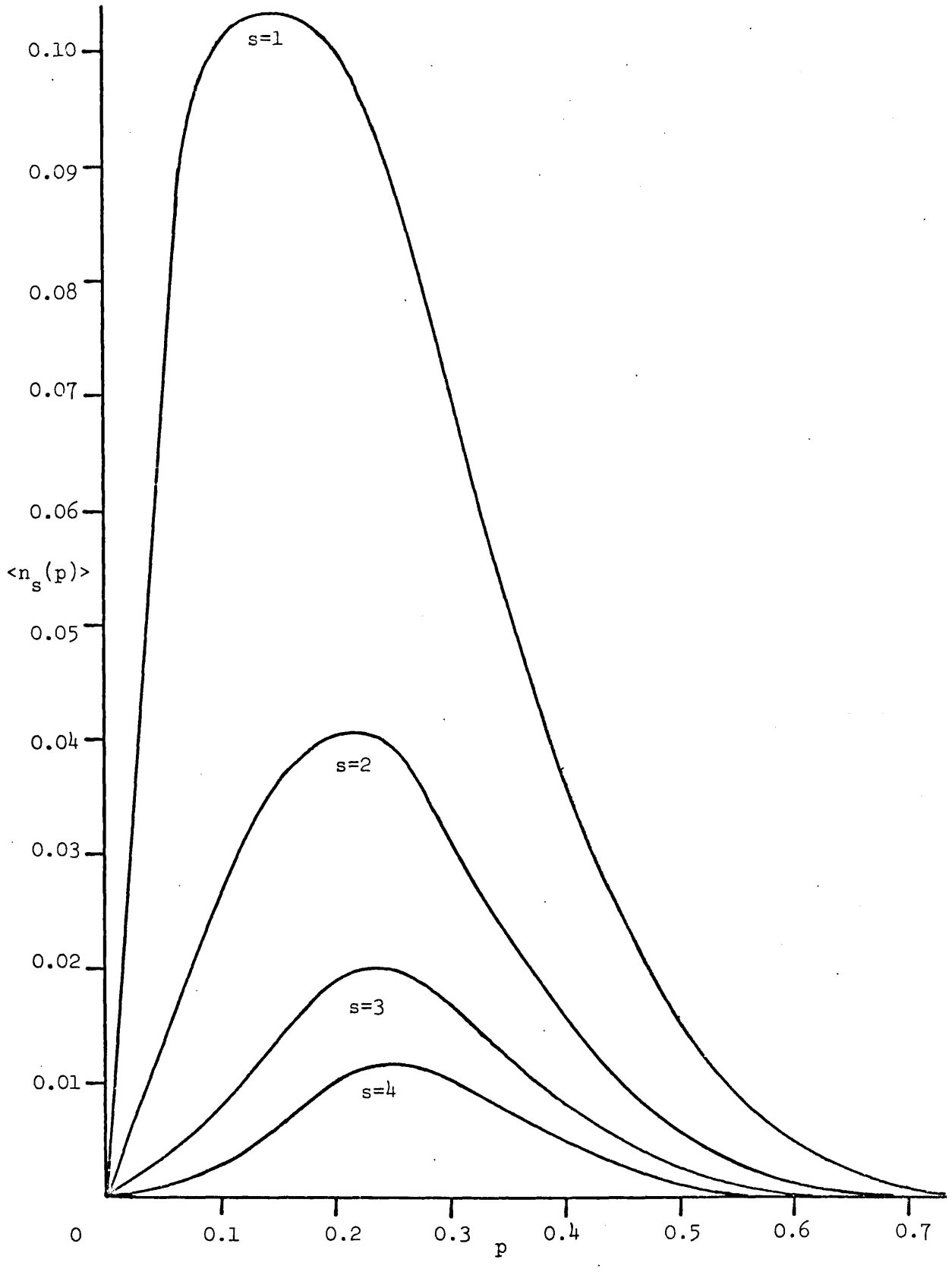


Fig 1.7 Variation of the mean number of clusters, of a given size, with p on the $\sigma = 3$ Bethe Lattice.

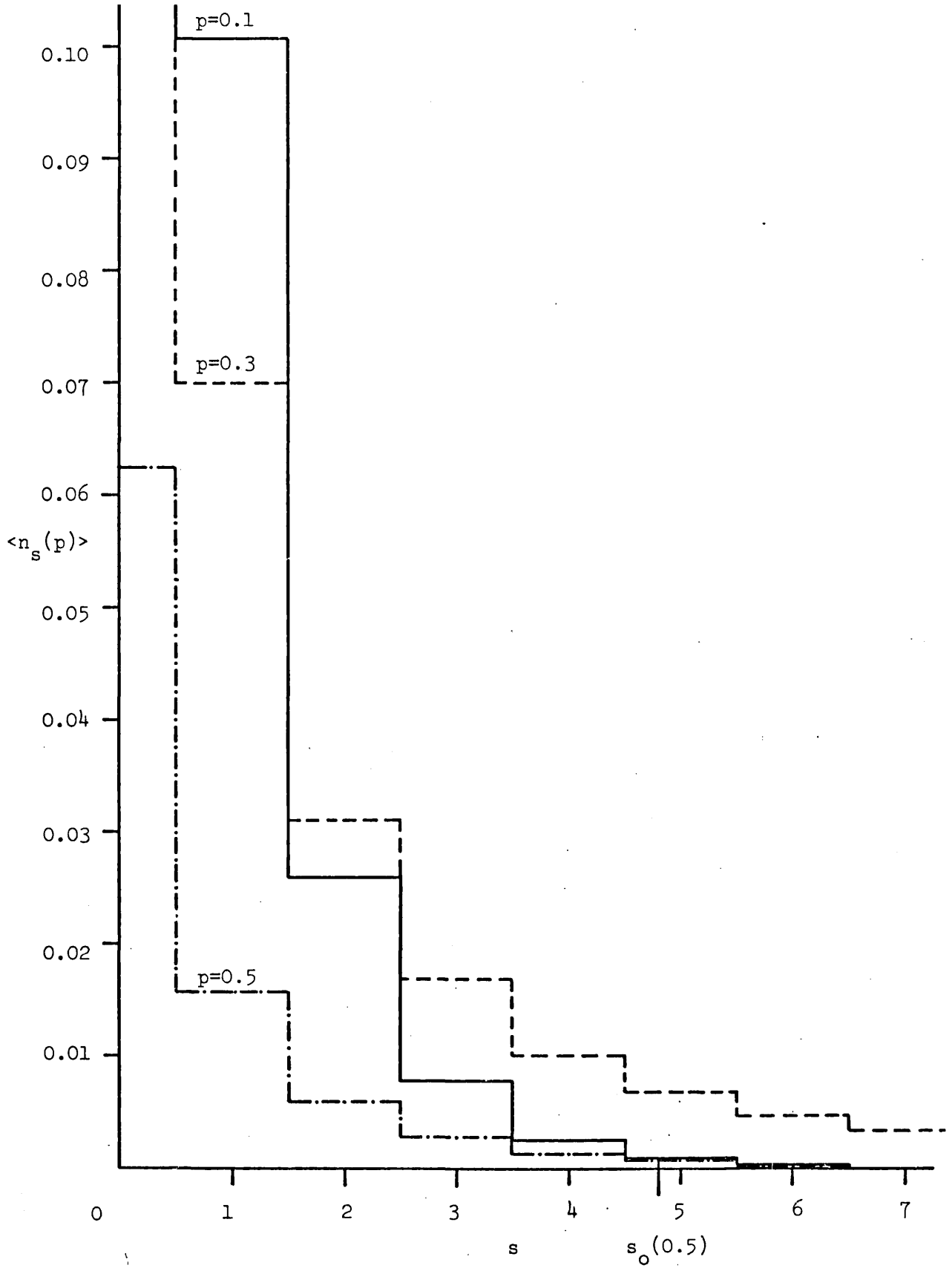


Fig. 1.8 Variation of the mean number of clusters $\langle n_s(p) \rangle$ with s for a given value of p .

where

$$\mu(p) = 1 - A|p-p_c|^{\Delta} \qquad (1.32)$$

A is a constant and Δ is the gap index (see later). From (1.31) and (1.32)

$$\langle n_s(p_c)\rangle \sim s^{-g} \quad . \qquad (1.33)$$

On the square lattice (bond problem) $\langle n_s(p)\rangle$ is known up to $s = 10$. Using (1.33) we have estimated the value of g, obtaining $g = 2$, and hence derived a value for the remainder of the mean number of clusters defined by $R = c \sum_{s>10} s^{-g}$ where c is a constant.

Once R was known we estimated a value for $k(p_c,L)$,

$$k(p_c,L) = \sum_{s=1}^{10} \langle n_s(p_c)\rangle + R \quad ,$$

which was accurate to within four decimal places of the result obtained by Temperley.

If we write $\mu(p) = e^{-1/s_o(p)}$ in (1.31) we obtain

$$\langle n_s(p)\rangle \sim e^{-s/s_o(p)}\, s^{-g} \quad .$$

Now $s_o(p)$, for a given p, can be interpreted as a characteristic size or cut-off point. That is the probability of finding a cluster of size greater than $s_o(p)$, for a given p, is very small. (See Fig. 1.8.)

The n^{th} moment of the cluster distribution is defined as

$$M_n(p) = \sum_{s,w} s^n p^s q^w a_{s,w} \quad . \tag{1.34}$$

(In Fig. 1.9 we plot the mean size of cluster per site, for the Bethe lattice, as a function of p .) Now

$$M_n(p) \sim |p-p_c|^{-[\gamma+(n-2)\Delta]} \tag{1.35}$$

(see chapter 4) where γ is the critical exponent of the mean size of clusters and Δ is the gap index.

Since there are very few exact calculations of the variation of the moment distributions near p_c we shall be concerned in calculating values for the critical exponents, defined above, and establishing the relation $\gamma = (3-g)\Delta$ between them. We also estimate values of p_c for various two and three dimensional lattices.

1.3 Derivation of Cluster Expansions [6]

The problem is initially formulated for a finite linear graph G using the terminology of graph theory [7]. Only the site problem will be considered since the equivalent results for the bond problem can nearly always be obtained by a simple change of variable. Two methods will be described to obtain the mean size of clusters expansion.

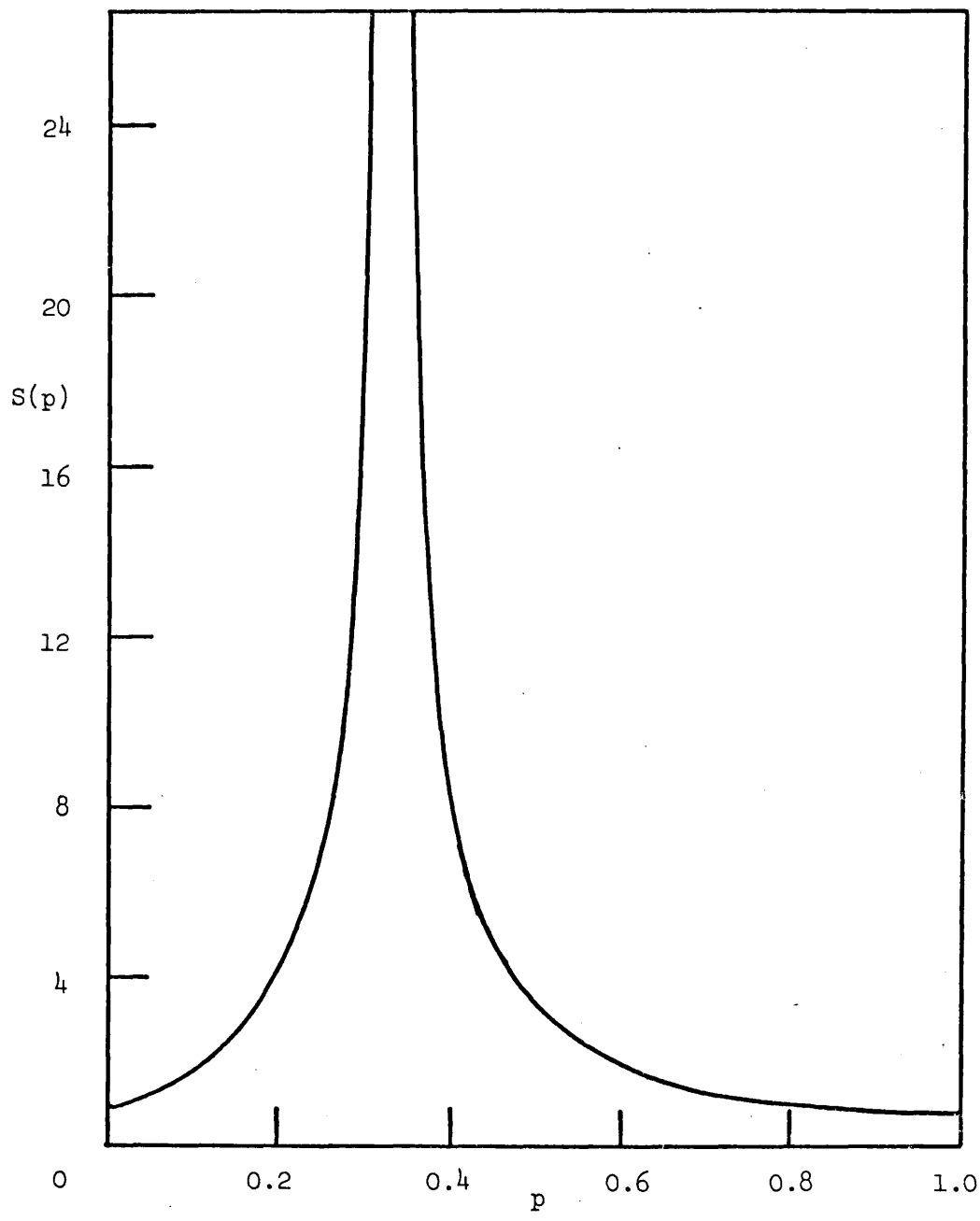


Fig. 1.9 Variation of the mean size of clusters with p for the $\sigma = 3$ Bethe Lattice.

(a) The Perimeter Method

To formulate the problem more clearly the occupied vertices will be termed black while the unoccupied vertices will be called white. As before (1.25) we write the mean number of black clusters as

$$K(p;G) = \sum_{s,w} K_{s,w}(G)p^s(1-p)^w \qquad (1.36)$$

where $K_{s,w}(G)$ is the number of connected section graphs of G with s vertices the corresponding clusters of which have perimeter w.

The mean number of clusters of size s is given by

$$K_s(p;G) = \sum_{w} K_{s,w}p^s(1-p)^w \quad . \qquad (1.37)$$

In terms of which the mean number of black vertices may be written

$$V(G)p = \sum_{s} sK_s(p;G) \qquad (1.38)$$

where $V(G)$ is the number of vertices in the graph G. The mean size of black clusters is usually defined by

$$S(p;G) = (\sum_{s} s^2K_s(p;G))/V(G)p \quad . \qquad (1.39)$$

Note. The higher moment distributions are obtained by simply replacing s^2 in (1.39) by s^n.

The mean number of black clusters of size s may be written as a polynomial in p of degree at most $V(G)$

$$K_s(p;G) = \sum_r A_{s,r}(G)p^r \qquad (1.40)$$

where

$$A_{s,r}(G) = (-1)^{r-s}\sum_w \binom{w}{r-s} K_{s,w}(G) \quad s \leq r$$

$$= 0 \qquad\qquad\qquad\qquad s > r \qquad (1.41)$$

The perimeter method is to determine the values of $A_{s,r}$ by inspection of the graph G and hence to obtain the mean size expansion $S(p;G)$ as a polynomial in p. We shall see in section 1.4 that this method, on a lattice, yields a power series in p which is only expected to converge for $p < p_c$.

(b) The Linked Cluster Expansion

Only a brief description will be given here of the linked cluster expansion technique [6] as the method is used only once to derive a series on the honeycomb lattice. (See appendix III). It is possible to write the n^{th} moment of the cluster size as a polynomial in p

$$M_n(p;G) = \sum_m [C_m;G]M_n(C_m)p^{s_m} \qquad (1.42)$$

where $[C_m;G]$ is the strong lattice constant of the graph C_m in G and is defined as the number of section graphs of G isomorphic with C_m. $M_n(C_m)$ is the strong n^{th} moment weight factor for the graph C_m and is independant of G.

The main difficulty with this method lies in the enumeration of the $M_n(C_m)$ and we consider two methods of obtaining the

strong second moment weight factors. The first makes use of the fact that

$$M_2(1,C) = V(C)^2 \tag{1.43}$$

where C is any connected graph.

Combining (1.43) with (1.42) gives

$$\sum_m [C_m;C] M_n(C_m) = V(C)^2 \quad . \tag{1.44}$$

The second method exploits the connection of $M_2(p;G)$ with the pair connectivity. It is shown in [9] and [10] that

$$\begin{aligned} M_2(C) &= 2\sum_t D(C_t^{ii}) \qquad V(C) > 1 \\ &= 1 \qquad\qquad\quad V(C) = 1 \quad . \end{aligned} \tag{1.45}$$

Here C_t^{ii} is the t^{th} two rooted graph obtained by rooting two of the vertices of C and $D(C_t^{ii})$ is the strong pair connectivity weight. There are altogether $\frac{1}{2}V(C)\{V(C)-1\}$ terms in the summation. The strong pair connectivity weights are given in terms of the strong mean number weights [11] by

$$D(C^{ii}) = K(C') - K(C) \qquad V(C^{ii}) > 2$$

or (1.46)

$$D(C^{ii}) = K(C^{(n)}) \qquad n \geq 2 \ , \ V(C^{ii}) > 2$$

where $C^{(n)}$ is the unrooted graph obtained from the two rooted graph C^{ii} by inserting a chain of n edges having the root

points as terminal vertices and treating the root points as ordinary vertices. Also $C' = C^{(1)}$ and C is the unrooted graph obtained from C^{ii} by treating the root points as ordinary vertices.

1.4 Low Density Series Expansions for Bond and Site Problems on a Crystal Lattice.

In order to apply the results of the previous section we suppose that G_n is a member of a sequence of finite graphs which tend to L, the infinite lattice, as n tends to infinity.

The mean size of black clusters as defined in (1.39) needs re-defining for the infinite graph L

$$pS(p;L) = \sum_{s=1}^{\infty} s^2 \langle n_s(p) \rangle \qquad (1.47)$$

where $\langle n_s(p) \rangle$ is the specific mean number of clusters of size s.

It is a property of crystal lattices that if only pairs of sites which are separated by a finite distance are taken as the edges of L then a finite section graph of L will have a finite perimeter. It follows from (1.37) that if s is finite than $\langle n_s(p) \rangle$ is a polynomial in p which vanishes for real p in the range $0 \leq p \leq 1$ only at $p=0$ and $p=1$, except when the number of edges $\ell=0$, and therefore has a single maximum in this region. It will be supposed that the infinite sum (1.47) converges

in this region except at a single point called the critical probability. In the region above the critical probability (i.e. $p > p_c$) $S(p;L)$ represents the mean size of finite black clusters. On all the lattices investigated (see chapter 3) the coefficients of the power series expansion derived from (1.47) are all positive and they have been used as a basis for the determination of the critical probability [12]-[19].

1.5 Extension of the Low Density Series Expansions for the Mean Size of Clusters and Higher Moments

If we expand (1.47) as a power series the n^{th} moment of the cluster size may be written

$$M_n(p;L) = 1 + \sum_{r=1}^{\infty} S_r(L)p^r \qquad (1.48)$$

where

$$S_{r-1}(L) = \sum_{s=1}^{r} s^n a_{s,r}(L) \qquad (1.49)$$

where

$$a_{s,r}(L) = (-1)^{r-s}\sum_{w}(r^w_s)k_{s,w}(G) \quad s \leq r$$

$$= 0 \quad s > r \qquad (1.50)$$

and $a_{s,r}(L)$ forms an infinite matrix $a(L)$.

Suppose the first s columns of $a(L)$ are known then $S_1(L)$ through to $S_{s-1}(L)$ may be obtained.

The specific mean number of black vertices which are contained in finite black clusters is equal to p provided $p < p_c$. Using

the perimeter method to derive a low density expansion for the specific mean number of black vertices, $M_1(p;L)$ all the coefficients other than the first must be zero so that

$$\sum_{s=1}^{r} s\, a_{s,r}(L) = 0 \qquad r > 1 \quad . \tag{1.51}$$

This enables $S_1(L)$ through to $S_s(L)$ to be obtained since eliminating $a_{r,r}(L)$ from (1.49) and (1.51) gives

$$S_{r-1}(L) = \sum_{s=1}^{r-1} s(s^{n-1} - r^{n-1}) a_{s,r}(L) \quad . \tag{1.52}$$

Thus an extra term is obtained without deriving any further information.

A low density expansion may also be obtained for the specific mean number of black clusters

$$k(p;L) = \sum_{r=1}^{\infty} k_r(L) p^r \tag{1.53}$$

where

$$k_r(L) = \sum_{s=1}^{r} a_{s,r}(L) \quad . \tag{1.54}$$

The coefficients $k_r(L)$ may be obtained independently using the linked cluster method. Because the mean number weights are zero for articulated graphs (see appendix V for definition) only multiply connected graphs contribute to $k_r(L)$. Consequently the mean number expansion is much easier to determine than the higher moment expansions. Solving (1.51) and (1.54) for $a_{r-1,r}(L)$ and $a_{r,r}(L)$ and substituting in (1.49) gives

$$S_{r-1}(L) = \sum_{s=1}^{r-2} \{[s^n+(r-1)^n(s-r)+r^n(r-s-1)]a_{s,r}(L)\}$$

$$+[(r-1)^n r-(r-1)r^n]k_r(L) \quad . \tag{1.55}$$

Thus using the same number of polynomials together with (1.55) allows the mean size of coefficients through $S_{s+1}(L)$ to be obtained.

For a lattice and its corresponding matching lattice it can be shown that [20]

$$k(p;L) = \phi(p) + k(q;L^*) \tag{1.56}$$

and

$$k(p;L^*) = \phi^*(p) + k(q;L) \quad . \tag{1.57}$$

Effectively this states that at density p the mean number of black clusters on L differs from the mean number of white clusters on L^* by $\phi(p)$. Similarly the mean number of black clusters on L^* differs from the mean number of white clusters on L by $\phi^*(p)$.

When working with the matching lattices it is easier to derive $k_r(L)$ using the high density series in q on the corresponding lattice, e.g. if $k_r(L)$ is required on the honeycomb matching lattice it is easier to derive the coefficient of q^r on the plane honeycomb lattice which is identical providing $r > 6$.

Using the above method the mean number series through $k_9(L)$

was derived on the honeycomb matching lattice. (This series is listed in appendix III.)

1.6 Derivation of a 'Bond' series from a 'Site' series

From the definition of a subgraph and a section graph [22] (see appendix V) we see that all subgraphs are contained in section graphs, i.e. a subgraph is obtained by deleting edges from the appropriate section graph. It is this fact which enables a bond series to be derived from a site series using the Yield Factor technique. We define the yield factor of a graph $G = (V,E)$ to be

$$Y_G(q) = \sum_{\substack{E' \subseteq E \\ \bar{E}' = E}} q^{|E-E'|} \qquad (1.58)$$

where $\bar{E}'$ denotes the bond closure of E. (See appendix V.)

If a section graph G has a 'site' count a_s, ℓ edges and a bond perimeter w then this graph makes a contribution to the bond series of

$$a_s p^{\ell} q^{w} Y_G(q) \quad .$$

Consequently if all the section graphs up to n sites are known on a lattice then the bond series can be obtained up to p^{n-1}.

In appendix IV the yield factors of graphs, up to seven sites, on the F.C.C. lattice are listed. To obtain the seven bond

perimeter polynomial it was then only necessary to count, for the bond problem, all seven bond trees with their perimeter distribution. To extend the mean size series by one term the mean number coefficient for nine bond graphs was calculated.

To obtain the site count of a graph from the bond count we use the Möbius inversion method [23] and [24]. If the site count of a graph G is $a_s(V,E)$ then the bond count is

$$a_b(V,E) = \sum_{E'} \xi(E,E') a_s(V,E') \tag{1.59}$$

where the sum is over a complete list of subgraphs of $|V| = s$ vertices and

$$\xi(E,E') = \begin{cases} 1 & \text{if } E \subseteq E' \\ 0 & \text{otherwise} \end{cases} .$$

Inverting (1.59) we obtain

$$a_s(V,E) = \sum_{E'} \mu(E',E) a_b(V,E') \tag{1.60}$$

where μ is the inverse of ξ and is known as the Möbius function. In this case μ is known to be [24]

$$\mu(E',E) = \begin{cases} (-1)^{|E-E'|} & \text{if } E' \subseteq E \\ 0 & \text{otherwise} \end{cases} .$$

In appendix II, μ is derived for a lattice [23] defined such that no graph in the lattice has less than one multiply connected block.

1.7 Thesis Description

So far we have described methods used to derive site and bond series for a crystal lattice. We endeavour in the chapters that follow to determine how the functions, represented by these series, vary near the critical point p_c. We assume that the n^{th} moment, near p_c, varies as $(1 - p/p_c)^{-c_n}$, where c_n is the critical point exponent of the n^{th} moment. We derive values for c_n and obtain relationships between them. The series methods however only provide approximate results and so in chapter 2 we investigate the Bethe lattice. (See Fig. 1.6.)

We obtain exact values for the exponents γ, Δ and g, and show that they satisfy the relation $\gamma = (3-g)\Delta$.

In chapter 3 we introduce the ratio method. This is used to derive the critical probability p_c from the series obtained using the perimeter method. Approximate values for some of the critical exponents are obtained and relations between them investigated. Unfortunately to obtain some of the results it has been necessary to use series which do not have enough terms, consequently many of the results have large error bounds. To derive extra terms demands an unreasonable amount of work compared with the extra accuracy gained, since one or even two more terms in a series make very little difference to the error bounds. Even once the lattice configurations are known the lattice count and perimeter of each graph has to be determined and even with the aid of computers the higher order terms cannot be obtained using the

'counting' techniques now available. It is necessary to determine a different method by which these series may be obtained. The linked cluster technique seemed to provide a solution since it reduced the total number of graphs to be counted, i.e. all trees were eliminated. Unfortunately, for any but the most simple lattices, it has proved equally difficult to obtain the weight factors for the graphs used.

In chapter 4 we derive the scaling laws for percolation processes. Initially the results are obtained exactly using the Bethe lattice and then generalised to include two and three dimensional lattices. We have only really investigated the mean number series for the F.C.C. lattice (site problem) as this seemed to provide the best results for the number of terms available. More investigation is required in this field, for example, other mean number series on different lattices, the F.C.C. bond problem particularly, should prove amenable to the same treatment. (See chapter 4.) The Padé approximant method should also prove useful in investigating the mean number series on lattices for which the Nevilles table (see chapter 3) in the above method does not converge.

In chapter 5 we calculate the critical exponent δ which occurs in the case of the dilute ferromagnet. δ describes the variation of the magnetisation with the field near the critical point $T_c(p)$, i.e. $M \sim H^{1/\delta}$. We have succeeded in calculating δ at the two end points of the $T_c(p)$ vs p curve (see Fig. 1.4,

section 1.1) but at no other point on it. It is important to note that the two values of δ are different and therefore the index must change its value somewhere on the curve. We tried to derive δ at a general point on the curve using a method essentially similar to that used to derive δ at $T_c(1)$, (see chapter 5 section 2). Unfortunately this failed because each graph contributed a different term to the partition function Z and therefore the total contribution from all graphs could not be obtained.

Chapter 6 is divorced from the preceeding chapters in that no critical exponents are calculated. Rather we establish a relationship, conjectured by G.A. Baker Jr. and J.W. Essam, between the k weight of a graph and the number of blocks of the graph.

Chapter 2 Derivation of, and relationship between, the critical exponents γ , Δ and g for the Bethe lattice

2.1 Relationship between critical exponents

Initially we derive a relationship between γ , Δ and g which holds for all two and three dimensional lattices as well as the Bethe lattice. The result is not rigorously proved however since equation (2.19) involves the summation of a limiting procedure.

The n^{th} moment of the cluster size distribution varies as:

$$M_n(p) \sim A_n(1-p/p_c)^{-\gamma-(n-2)\Delta} \tag{2.11}$$

we define

$$f(\lambda,p) = \sum_{r=0}^{\infty} \langle n_r \rangle \lambda^r \tag{2.12}$$

$$f(\lambda,p_c) = \sum_{r=0}^{\infty} \langle n_r \rangle_{p=p_c} \lambda^r \tag{2.13}$$

where:

p_c is the critical probability for the lattice and $\langle n_r \rangle$ is the mean number of clusters of r sites (bonds).

We show in section 4.2 that $\langle n_r \rangle_{p=p_c} \sim \frac{A}{r^g}$ then

$$f(\lambda,p_c) - f(1,p_c) \sim A(1-\lambda)^{g-1} \quad . \tag{2.14}$$

Expanding $f(\lambda,p)$ in a power series about $\lambda=1$ gives

$$f(\lambda,p) = \sum_{n=0}^{\infty} \frac{f^{(n)}(1,p)}{n!} (\lambda-1)^n \quad . \tag{2.15}$$

Let $\mu = \log\lambda$

then $d\mu = \frac{1}{\lambda} d\lambda$

and $$M_n(p) = \frac{\partial^n}{\partial \mu^n} \bar{f}(\mu,p)\Big|_{\mu=0} \tag{2.16}$$

where $$\bar{f}(\mu,p) = \sum_{n=0}^{\infty} \frac{\bar{f}^{(n)}(0,p)}{n!} \mu^n \tag{2.17}$$

$$= \sum_{n=0}^{\infty} \frac{M_n(p)}{n!} \mu^n \tag{2.18}$$

$$= \sum_{n=0}^{\infty} \frac{A_n}{n!} (1-p/p_c)^{-\gamma-(n-2)\Delta} \mu^n \tag{2.19}$$

$$= (1-p/p_c)^{-\gamma+2\Delta} F\left(\frac{\mu}{(1-p/p_c)^{\Delta}}\right) \tag{2.20}$$

$$\bar{f}(\mu,p) = \phi^{-\gamma+2\Delta} F\left(\frac{\mu}{\phi^{\Delta}}\right)$$

$$= \mu^{\frac{\gamma}{\Delta}+2} \cdot \frac{\phi^{-\gamma+2\Delta}}{\mu^{\frac{\gamma}{\Delta}+2}} F(x) \qquad x = \frac{\mu}{\phi^{\Delta}}$$

$$\bar{f}(\mu,p) = \mu^{-\frac{\gamma}{\Delta}+2} G(x) \tag{2.21}$$

hence $$\bar{f}(\mu,p_c) \sim \mu^{-\frac{\gamma}{\Delta}+2} \sim (1-\lambda)^{\frac{\gamma}{\Delta}+2}$$

therefore $g - 1 = -\frac{\gamma}{\Delta} + 2$

$$g = 3 - \frac{\gamma}{\Delta} \quad . \tag{2.22}$$

2.2 Calculation of γ and Δ for the Bethe lattices

We now consider the values of the above indices for the bond problem on the Bethe Lattices [27]. Following the methods used in [25] we write the configurational generating function as

$$K^B(x,y) = y^{\sigma+1} \sum_{s=0}^{\infty} b_s x^s y^{(\sigma-1)s} \tag{2.23}$$

where

$(\sigma-1)s + \sigma + 1$ is the perimeter of a cluster of s occupied bonds

b_s is the total number of s clusters (of bonds) per bond of the Bethe lattice.

The expansion (2.23) may be re-written in terms of the fundamental Bethe lattice generating function

$$B_\sigma(Z) = \sum_{s=0}^{\infty} b_s Z^s$$

as

$$K^B(x,y) = y^{\sigma+1} B_\sigma(Z)$$

where

$$Z(x,y) = xy^{\sigma-1}$$

now

$$A(x,y) = x \frac{\partial}{\partial x} \{K^B(x,y)\}$$

$$= xy^{2\sigma} B'_\sigma(Z)$$

where the prime denotes differentiation with respect to Z .

A fundamental identity is that for $p < p_c$ $A(p,q) \equiv p$. Thus, if

$$z = z(p) = Z(p,q) = p(1-p)^{\sigma-1} \tag{2.24}$$

the generating function must satisfy

$$B'_\sigma[z(p)] = G(p) = (1-p)^{-2\sigma} \tag{2.25}$$

for small enough p . Now $B_\sigma(z)$ is a function only of z , but z is defined by (2.24) as a function of p for all p . To a given value of z , however, correspond two values of p , one of which tends to zero with z while the other tends to unity. Consequently if we define $p^*(p)$ to be the root of the equation

$$p^*(1-p^*)^{\sigma-1} = p(1-p)^{\sigma-1} = z$$

which vanishes continuously with z , we may re-write (2.25) as

$$G(p) = [1 - p^*(p)]^{-2\sigma}$$

hence we may write

$$B'_\sigma(Z) = [1 - X(Z)]^{-2\sigma}$$

where $X(Z) = X(x,y)$ is the root of

$$X(1 - X)^{\sigma-1} = Z = xy^{\sigma-1}$$

which vanishes with Z .

Now $$S(p) = \left[x \frac{\partial}{\partial x} \ln A(x,y) \right]_{x=p,y=q}$$

for all values of p .

$$S(p) = 1 + xy^{\sigma-1} \frac{B''_\sigma(Z)}{(1-X)^{-2\sigma}} \Bigg|_{x=p,y=q,X=p^*(p)}$$

where

$$B''_\sigma(Z) = \frac{2\sigma}{(1-X)^{3\sigma-1}(1-\sigma X)}$$

hence

$$S(p) = \frac{1 + \sigma p^*}{1 - \sigma p^*} \qquad (2.26)$$

near $p = p_c$

$$p^*(p) \tilde{\sim} p_c - |p-p_c|$$

so that the mean cluster size becomes hyperbolically infinite as

$$S(p) \sim \frac{2}{(1-p/p_c)}$$

hence $\gamma = 1$ for the Bethe lattice.

The third moment of the cluster size distribution is defined as

$$M_3(p) \equiv \frac{1}{A(x,y)} \left(x\frac{\partial}{\partial x}\right)\left(x\frac{\partial A(x,y)}{\partial x}\right)$$

$$= \frac{(1-X)^{2\sigma}}{xy^{2\sigma}} \{xy^{2\sigma}B'_\sigma(Z) + x^2y^{3\sigma-1}B''_\sigma(Z)$$

$$+ 2x^2y^{3\sigma-1}B''_\sigma(Z) + x^3y^{4\sigma-2}B'''_\sigma(Z)\}$$

$$= 1 + \frac{6\sigma X}{(1-\sigma X)} + 2\sigma X^2 \frac{(4\sigma-3\sigma^2X-1)}{(1-\sigma X)^3}$$

$$M_3(p) = \frac{1 + 3\sigma p^* - \sigma^2 p^{*2} - \sigma^3 p^{*3} - 2\sigma p^{*2}}{(1 - \sigma p^*)^3}$$

hence $M_3(p)$ becomes hyperbolically infinite as

$$M_3(p) \sim \frac{2 - 2/\sigma}{(1-p/p_c)^3}$$

hence $\Delta = 2$.

Using the relationship derived in (2.22) gives a value for g of $5/2$.

2.3 Proof that $g = 5/2$ for the Bethe lattice

Method 1.

If we assume that $\langle n_s \rangle_{p=p_c} \sim \frac{A}{s^g}$

then

$$\frac{\langle n_{s-1} \rangle_{p=p_c}}{\langle n_s \rangle} \sim 1 + g/s + \ldots \qquad (2.27)$$

from the equation (2.23)

$$\langle n_s \rangle = q^{\sigma+1} b_s p^s q^{(\sigma-1)s}$$

[25] shows that on the Bethe lattice $p_c = \frac{1}{\sigma}$

and

$$b_s = \frac{2(\sigma s+\sigma+1)!}{(s+1)(\sigma s+\sigma+1)(\sigma s+\sigma+1-s)!s!}$$

therefore

$$\frac{\langle n_{s-1} \rangle}{\langle n_s \rangle}\Bigg|_{p=p_c=\frac{1}{\sigma}} = \sigma\left(\frac{\sigma}{\sigma-1}\right)^{\sigma-1} \frac{(\sigma s)!(s+1)(\sigma s+\sigma+1-s)!}{(\sigma s+2-s)!\ \ (\sigma s+\sigma)!}$$

$$\frac{\langle n_{s-1} \rangle}{\langle n_s \rangle}\Bigg|_{p=\frac{1}{\sigma}} = \left(\frac{\sigma}{\sigma-1}\right)^{\sigma-1} \left\{\frac{[s(\sigma-1)+\sigma+1][s(\sigma-1)+\sigma]\ldots[s(\sigma-1)+3]}{[\sigma s+\sigma-1][\sigma s+\sigma-2]\ldots[\sigma s+1]}\right\}$$

hence dividing throughout by σs

$$\frac{\langle n_{s-1} \rangle}{\langle n_s \rangle}\Bigg|_{p=\frac{1}{\sigma}} \sim \left(\frac{\sigma}{\sigma-1}\right)^{\sigma-1} \left\{\left(\frac{\sigma-1}{\sigma}+\frac{\sigma+1}{\sigma s}\right)\left(\frac{\sigma-1}{\sigma}+\frac{\sigma}{\sigma s}\right)\ldots\left(\frac{\sigma-1}{\sigma}+\frac{3}{\sigma s}\right)\right.$$

$$\left. \times \left(1-\frac{\sigma-1}{\sigma s}\right)\left(1-\frac{\sigma-2}{\sigma s}\right)\ldots\left(1-\frac{1}{\sigma s}\right)\right\}$$

$$\sim \left(\frac{\sigma}{\sigma-1}\right)^{\sigma-1} \left\{\left[\left(\frac{\sigma-1}{\sigma}\right)^{\sigma-1} + \frac{1}{\sigma s}\left(\frac{\sigma-1}{\sigma}\right)^{\sigma-2}\left(\tfrac{1}{2}(\sigma+1)(\sigma+2)-3\right)\right]\right.$$

$$\left. \times \left[1-\frac{1}{\sigma s}\left(\tfrac{1}{2}\sigma(\sigma-1)\right)\right]\right\}$$

$$\sim \left[1+\frac{1}{2s(\sigma-1)}(\sigma-1)(\sigma+4)\right]\left[1-\frac{1}{2s}(\sigma-1)\right]$$

$$\sim 1+\frac{5}{2s}$$

hence from (2.27)

$$g = 5/2 \quad .$$

Method 2.

From [25] the Bethe lattice generating function

$$B_\sigma(Z) = \frac{1}{\sigma+1} \frac{[2 - (\sigma+1)X(Z)]}{[1-X(Z)]^{\sigma+1}} \quad . \tag{2.28}$$

At the critical point $X_c = \frac{1}{\sigma}$ and the value of Z has a maximum $Z_c = \frac{1}{\sigma^\sigma}(\sigma-1)^{\sigma-1}$

now $K^B(x,y) = y^{\sigma+1}B_\sigma(Z)$

but at $p = p_c$ the mean number function

$$K^B(p_c,\lambda) \sim (1 - \lambda)^{g-1} \qquad \text{where} \quad \lambda = \frac{Z}{Z_c}$$

hence we require an expansion of $B_\sigma(Z)$ in terms of Z/Z_c .

Since we are only concerned with positions very close to the critical point we write

$$X = X_c - \varepsilon$$

$$Z = (X_c - \varepsilon)(1 - X_c + \varepsilon)^{\sigma-1}$$

$$= X_c(1 - X_c)^{\sigma-1}(1 - \frac{\varepsilon}{X_c})(1 + \frac{\varepsilon}{1-X_c})^{\sigma-1}$$

$$Z = Z_c(1 - \sigma\varepsilon)(1 + \frac{\sigma\varepsilon}{\sigma-1})^{\sigma-1} \quad . \tag{2.29}$$

Expanding (2.29) in powers of $\frac{\sigma\varepsilon}{\sigma-1}$ gives

$$Z = Z_c\left(1 - \frac{\sigma^3\varepsilon^2}{2(\sigma-1)} - \frac{\sigma^4(\sigma-2)\varepsilon^3}{3(\sigma-1)^2} + \ldots\ldots\right)$$

$$Z_c - Z = Z_c \cdot \tfrac{1}{2}\,\frac{\sigma^3\varepsilon^2}{(\sigma-1)}\left\{1 + \frac{2}{3}\,\frac{\sigma(\sigma-2)\varepsilon}{(\sigma-1)} + \ldots\ldots\right\}$$

hence

$$\varepsilon^2 = \frac{2(\sigma-1)}{\sigma^3}[1-Z/Z_c]\left\{1 - \frac{2}{3}\,\frac{\sigma(\sigma-2)}{(\sigma-1)}\left[\frac{2(\sigma-1)}{\sigma^3}\right]^{\frac{1}{2}} \times (1-Z/Z_c)^{\frac{1}{2}}\right\} .$$

Substituting the values for X into (2.28) gives

$$B_\sigma(Z) = \frac{1}{(\sigma+1)}\,\frac{(2-[\sigma+1]X_c)}{(1-X_c)^{\sigma+1}}\,(1 + \frac{\sigma(\sigma+1)\varepsilon}{(\sigma-1)})(1 + \frac{\sigma\varepsilon}{(\sigma-1)})^{-(\sigma+1)}$$

$$= B_c(1 + \frac{\sigma(\sigma+1)\varepsilon}{(\sigma-1)})\{1 - \frac{\sigma(\sigma+1)\varepsilon}{(\sigma-1)} + \frac{\sigma^2(\sigma+1)(\sigma+2)\varepsilon^2}{2(\sigma-1)^2} - \frac{\sigma^3(\sigma+1)(\sigma+2)(\sigma+3)\varepsilon^3}{6(\sigma-1)^3} + \ldots\ldots\}$$

$$= B_c\left(1 - \frac{\sigma^3(\sigma+1)\varepsilon^2}{2(\sigma-1)^2} + \frac{\sigma^4(\sigma+1)(\sigma+2)\varepsilon^3}{3(\sigma-1)^3} + \ldots\ldots\right) .$$

Replacing ε by the value previously derived gives

$$B_\sigma(Z) = B_c\{1 - \frac{(\sigma+1)}{(\sigma-1)}(1-Z/Z_c) + \frac{8\sigma^3}{3}\,\frac{(\sigma+1)}{(\sigma-1)^2}\left(\frac{2(\sigma-1)}{\sigma^3}\right)^{\frac{1}{2}} \times (1-Z/Z_c)^{3/2} + \ldots\ldots\} \qquad (2.30)$$

hence

$$K(p_c,\lambda) \sim A(1-\lambda)^{3/2} \qquad (2.31)$$

therefore $g - 1 = 3/2$ giving $g = 5/2$.

To check that the value of the constant A derived was correct, thus indicating that the method had been carried out correctly, the function $B_\sigma(Z)$ was calculated exactly for $\sigma = 3$.

2.4 Calculation of $B_3(Z)$

$$B_3(Z) = \frac{1}{2}\frac{(1 - 2X)}{(1 - X)^4} \quad . \tag{2.32}$$

To obtain a solution for $B_3(Z)$ in terms of Z we require X as a function of Z now

$$Z = X(1 - X)^2$$

$$X^3 - 2X^2 + X - Z = 0 \quad . \tag{2.33}$$

From the standard method for solving a cubic equation given in [26] we obtain the three roots of (2.32).

$$X_1 = (s_1 + s_2) + \frac{2}{3}$$

real for all values of Z

gives X_1 in the range

$X_1 \leq 0$

$\frac{1}{3} < X_1 < 1$

$X_1 \geq \frac{4}{3}$

$$X_2 = -\tfrac{1}{2}(s_1+s_2)+\frac{2}{3} + \frac{i\sqrt{3}}{2}(s_1-s_2)$$

real for $0 \leq Z \leq \frac{4}{27}$

gives X_2 in the range

$0 < X_2 \leq \frac{1}{3}$

Also $X_2 = 1$

$$X_3 = -\tfrac{1}{2}(s_1+s_2)+\frac{2}{3} - \frac{i\sqrt{3}}{2}(s_1-s_2) \quad \text{real for} \quad 0 \leq Z \leq \frac{4}{27}$$

gives X_3 in the range

$$1 \leq X_3 < \frac{4}{3}$$

Also $X_3 = \frac{1}{3}$

where

$$s_1 = [Z/2 - 1/27 + (Z^2/4 - Z/27)^{\frac{1}{2}}]^{1/3}$$

$$s_2 \quad [Z/2 - 1/27 - (Z^2/4 - Z/27)^{\frac{1}{2}}]^{1/3} \quad .$$

The root which is required in this particular case is X_2 since this is the root which decreases with Z .

X_2 will now be written as X .

$$X^2 = \frac{4}{9} + \frac{1}{4}(s_1+s_2)^2 - \frac{3}{4}(s_1-s_2)^2 - \frac{2}{3}(s_1+s_2)$$

$$+ \frac{2i\sqrt{3}}{3}(s_1-s_2) - \frac{i\sqrt{3}}{2}(s_1^2-s_2^2)$$

$$X^2(1-2X) = -2Z - \frac{2}{3} + (s_1+s_2) + \frac{2}{3}(s_1^2+s_2^2)$$

$$+ \frac{3i\sqrt{3}}{2}(s_1^2-s_2^2) + i\sqrt{3}(s_1-s_2) \quad .$$

In this case $Z_c = \frac{4}{27}$

therefore $Z = \frac{4}{27}\lambda$.

Substituting these values into (2.31) gives

$$B_3(\lambda) = \frac{27^2}{32\lambda^2}\left\{-\frac{8\lambda}{27} - \frac{2}{3} + \frac{2}{3}\left[2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}}\right]^{1/3}\right.$$

$$+ \frac{1}{3}\left[2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}}\right]^{2/3}$$

$$+ \frac{\sqrt{3}}{3}\, i\left[2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}}\right]^{2/3}$$

$$\left. - \frac{2\sqrt{3}}{3}\, i\left[2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}}\right]^{1/3}\right.$$

$$B_3(\lambda) = \frac{27}{32\lambda^2}\left\{-8\lambda-18+18\left[(2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}})^{1/3}\right.\right.$$

$$\left. + \frac{1}{2}(2\lambda-1+2(\lambda^2-\lambda)^{\frac{1}{2}})^{2/3}\right]$$

$$+ 18\sqrt{3}\, i\left[\tfrac{1}{2}(2\lambda-1+2i\lambda^{\frac{1}{2}}(1-\lambda)^{\frac{1}{2}})^{2/3}\right.$$

$$\left.\left. -(2\lambda-1+2i\lambda^{\frac{1}{2}}(1-\lambda)^{\frac{1}{2}})^{1/3}\right]\right\} \quad .$$

The real part of the first bracket gives an expansion in powers of $(1-\lambda)^n$.

While that of the second bracket gives an expansion in powers of $(1-\lambda)^{n+\frac{1}{2}}$ $n \neq 0$.

Considering the value for $B_3(\lambda)$ we see that the coefficient of $(1-\lambda)^{3/2}$ is $\frac{9\sqrt{3}}{2}$.

From equation (2.30) the coefficient of $(1-\lambda)^{3/2}$ is given by

$$B_c \frac{8}{3}\sigma^3 \frac{(\sigma+1)}{(\sigma-1)^2}\left\{\frac{2(\sigma-1)}{\sigma^3}\right\}^{\frac{1}{2}} = \frac{9\sqrt{3}}{2} \quad \text{for } \sigma = 3$$

hence we see that both results give the same value for the coefficient.

Chapter 3 Numerical estimates for critical probabilities and critical exponents for two and three dimensional lattices

3.1 Methods used to analyse series

In this chapter we derive certain mean size of cluster expansions, and higher moment expansions, for various lattices. The series were obtained using the perimeter method discussed in [27],[8],[20] and [6]. We have also used the linked cluster expansion technique to derive a series on the hexagonal lattice, the second moment weight factors being obtained from the pair connectivity weights. This series however has not been completely verified and is listed in appendix III.

The cluster size distributions for each lattice, contained in appendix I, were derived using a counting program to enumerate the complete list of seven site connected graphs. The majority of work was performed on the site problem where the known series were extended by a number of terms.

The mean size of cluster expansion can be defined in three ways for the site (bond) problem, (see [28])

$$\text{(i)} \quad pS(p) = \sum_s \sum_t a_{s,t} s^2 p^s q^t$$

$$\text{(ii)} \quad pS(p) = \sum_s \sum_t a_{s,t} s.e. p^s q^t$$

$$\text{(iii)} \quad pS(p) = \sum_s \sum_t a_{s,t} e^2 p^s q^t$$

where s is the size

t is the perimeter

e is the number of edges in the graph

$a_{s,t}$ is the count per site .

All three cases have been considered but (i) has proved to be the most useful. The series derived using (ii) and (iii) are listed in appendix III. The series (i) appear to converge more rapidly than either (ii) or (iii), see Fig. 3.1. Also methods are available which allow two extra terms to be derived for (i) and this is the real advantage over the other two series. This method has been extended as shown in section (1.4) to include the higher moment expansions.

If we expand the mean size of finite clusters in powers of p then:

$$S(p) = 1 + \sum_{n=1}^{\infty} a_n p^n \tag{3.10}$$

similarly for the higher moment expansions

$$M_3(p) = 1 + \sum_{n=1}^{\infty} b_n p^n \tag{3.11}$$

$$M_4(p) = 1 + \sum_{n=1}^{\infty} c_n p^n \quad . \tag{3.12}$$

If we assume as in [12] that $a_n \sim n^j p_c^{-n}$ then this implies that $S(p)$ has a singularity of the form $\frac{1}{(p_c-p)^\gamma}$ where

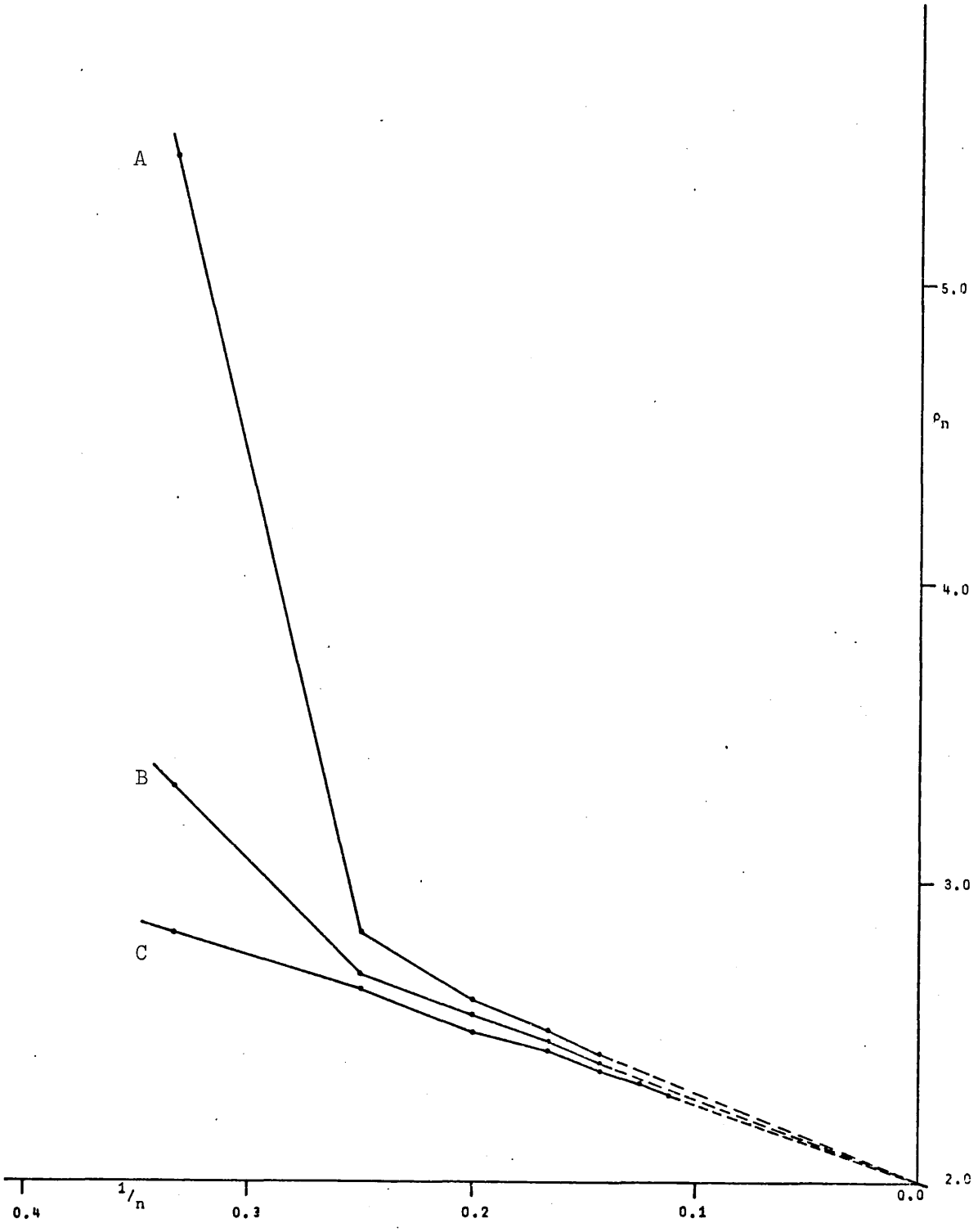


Fig. 3.1 Triangular Lattice site problem. Successive estimates for the critical percolation probability ($\rho_n \to 1/p_c$) plotted against $1/n$.
(A) Mean size expansion using e^2 (B) Mean size expansion using $s \times e$
(C) Mean size expansion using s^2 .

$\gamma = j+1$. Similarly for $M_3(p)$ and $M_4(p)$ except that a different value of j is expected.

All the methods which are now discussed will use the terminology of the mean size of cluster series. This is merely to avoid repetition as the analysis which follows is the same for the higher order moments.

We define, as in [12], the ratios of alternating terms as $\rho_n = (\frac{a_n}{a_{n-2}})^{\frac{1}{2}}$. These are tabulated for various lattices in tables (3.2), (3.5), (3.8), (3.11), (3.14). The function ρ_n is used rather than the direct ratios in an attempt to eliminate any oscillatory behaviour in the series. We plot ρ_n against $1/n$ in Figs. (3.2), (3.4), (3.6), (3.8), (3.10) and assume that $\lim_{n\to\infty} \rho_n = \rho = 1/p_c$. Values of the function $n\rho_n - (n-1)\rho_{n-1}$ were calculated and in this way estimates for p_c , on various two and three dimensional lattices, were made.

Once a value for p_c on each lattice is established successive estimates of j , defined by

$$j_n = n(\rho_n - \rho)/\rho \tag{3.13}$$

are calculated and these are presented in tables (3.3), (3.6), (3.9), (3.12), (3.15). The corresponding graphs are plotted in Figs. (3.3), (3.5), (3.7), (3.9), (3.11). It is assumed in calculating j_n for all three moments that all the series diverge

at the same critical point p_c . The numerical evidence, i.e. the ρ_n for each moment, seems to support this view.

When necessary we have used the Nevilles Table method to determine the intercept of the graphs of j_n against $1/n$. Here the "linear" extrapolants are given by $nj_n - (n-1)j_{n-1}$, the "quadratic" extrapolants q_n are given by $\frac{1}{2}[n\ell_n - (n-2)\ell_{n-1}]$, the "cubic" extrapolants by $\frac{1}{3}[nq_n - (n-3)q_{n-1}]$ and so on. The extrapolation is stopped when successive estimates cease to progress monotonically. As an example of the method we show in Table 3.0 the values derived for the fourth moment expansion on the hexagonal matching lattice site problem.

Table 3.0

n	j_n	ℓ_n	q_n	r_n	t_n
4	10.6145				
5	9.2506	3.7948			
6	8.5150	4.8372	6.9220	6.5078	
7	8.0675	5.3821	6.7445	6.5078	
8	7.7693	5.6818	6.5869	6.3081	6.1084

Once values of j for all three moments have been calculated it is possible to estimate a value for the gap index Δ .

From (2.11) $M_n(p) = A_n(1 - p/p_c)^{-\gamma-(n-2)\Delta}$ therefore if the indices of $S(p)$, $M_3(p)$ and $M_4(p)$ are: $j(a_n)+1$, $j(b_n)+1$, $j(c_n)+1$ respectively we see that

$$\Delta = j(b_n) - j(a_n)$$

and

$$\Delta = j(c_n) - j(b_n) \quad .$$

If any discrepancy has occurred between the two calculated values of Δ the average has been taken.

Then using the relationship $g = 3 - \gamma/\Delta$ we have estimated values of g .

3.2 Honeycomb Matching Lattice - site problem

Table 3.1

Coefficients for expansion of $S(p)$, $M_3(p)$ and $M_4(p)$. We quote the successive coefficients in tabular form

n	a_n	b_n	c_n
1	12	36	84
2	66	462	2046
3	312	3960	28848
4	1368	27576	300456
5	5685	168489	2577903
6	23034	943392	19343682
7	90288	4943826	131394240
8	350124	24666828	826812852

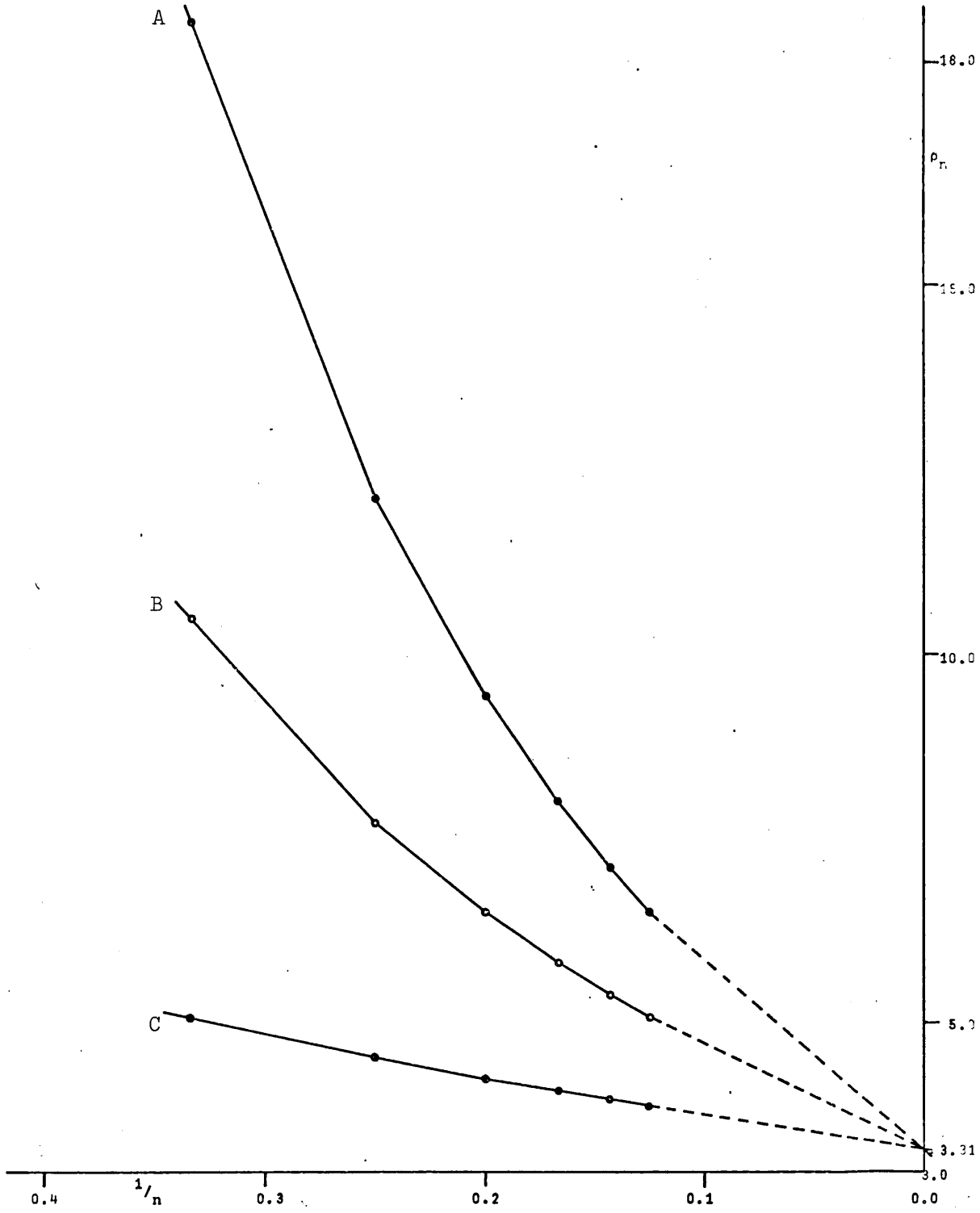


Fig. 3.2 Hexagonal Matching Lattice site problem. Successive estimates for the critical percolation probability ($\rho_n \to 1/p_c$) plotted against 1/n . (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

Table 3.2

Ratios of coefficients of expansion $\rho_n(a_n)$, $\rho_n(b_n)$ and $\rho_n(c_n)$

n	$\rho_n(a_n)$	$\rho_n(b_n)$	$\rho_n(c_n)$
3	5.0990	10.4881	18.5318
4	4.5527	7.7258	12.1182
5	4.2686	6.5229	9.4531
6	4.1034	5.8490	8.0238
7	3.9852	5.4168	7.1393
8	3.8988	5.1134	6.5378

From Fig. 3.2 the estimated value for p_c on this lattice is

$$p_c = 0.3015 \pm 0.001 \quad .$$

Table 3.3

Successive estimates of $j(a_n)$, $j(b_n)$ and $j(c_n)$ using the above value for p_c

n	$j_n(a_n)$	$j_n(b_n)$	$j_n(c_n)$
3	1.6121	6.4865	13.7620
4	1.4906	5.3173	10.6145
5	1.4350	4.8332	9.2506
6	1.4230	4.5808	8.5150
7	1.4108	4.4322	8.0675
8	1.4038	4.3335	7.7693

In order to estimate the values of j, from the above, graphs of j_n against $1/n$ were plotted, see Fig. 3.3, and where applicable a Nevilles Table was calculated for each set of values. This leads to estimations of j as

$$j(a_n) = 1.40 \pm 0.03$$

$$j(b_n) = 3.80 \pm 0.1$$

$$j(c_n) = 6.20 \pm 0.1 \quad .$$

This would indicate a gap index

$$\Delta = 2.4 \pm 0.2$$

and a value of g as $3 - \dfrac{2.4 \pm 0.03}{2.4 \pm 0.2}$.

It must be noted here that $g \geq 2$ hence the above error limits must be chosen to comply with this restriction.

Hence we can reduce the error limits on Δ to ,

$$\Delta = 2.4 \begin{matrix} + 0.2 \\ - 0.03 \end{matrix}$$

and

$$g = 2.0 + 0.1 \quad .$$

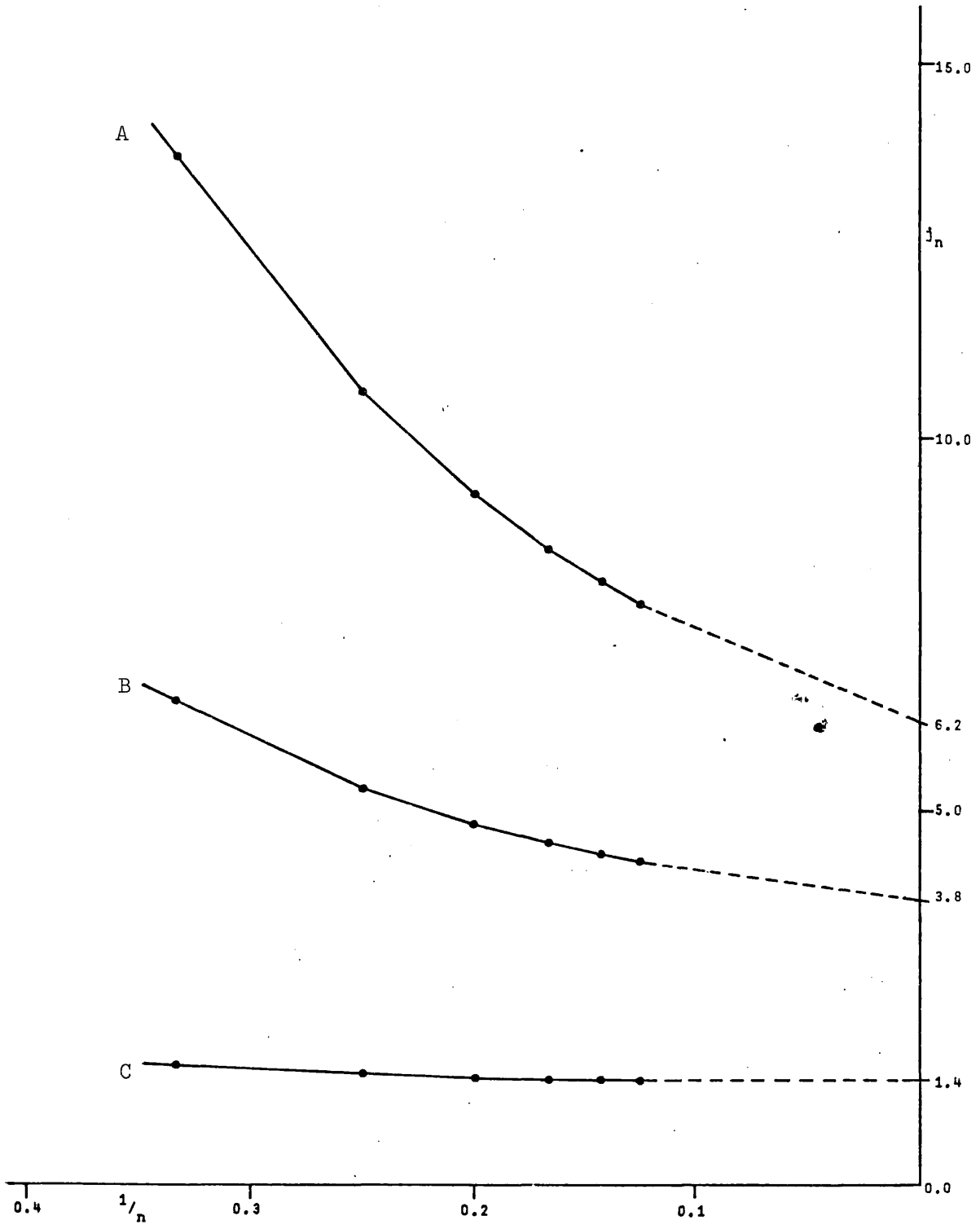


Fig. 3.3 Hexagonal Matching Lattice site problem. Successive estimates j_n for the index of the different moment expansions plotted against $1/n$. (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

3.3 Simple Quadratic Matching Lattice - site problem

Table 3.4

Coefficients for expansion of $S(p)$, $M_3(p)$ and $M_4(p)$.

We quote the successive coefficients in tabular form.

n	a_n	b_n	c_n
1	8	24	56
2	32	216	944
3	108	1308	9300
4	348	6516	68316
5	1068	28812	417924
6	3180	117216	2250924
7	9216	448152	11031480
8	26452	1636728	50294332

Table 3.5

Ratios of coefficients of $\rho_n(a_n)$, $\rho_n(b_n)$ and $\rho_n(c_n)$.

n	$\rho_n(a_n)$	$\rho_n(b_n)$	$\rho_n(c_n)$
3	3.6742	7.3824	12.8869
4	3.2977	5.4924	8.5070
5	3.1447	4.6933	6.7036
6	3.0229	4.2413	5.7401
7	2.9376	3.9439	5.1377
8	2.8841	3.7368	4.7269

From Fig. 3.4 the estimated value for p_c on this lattice is

$$p_c = 0.408 \pm 0.03 \quad .$$

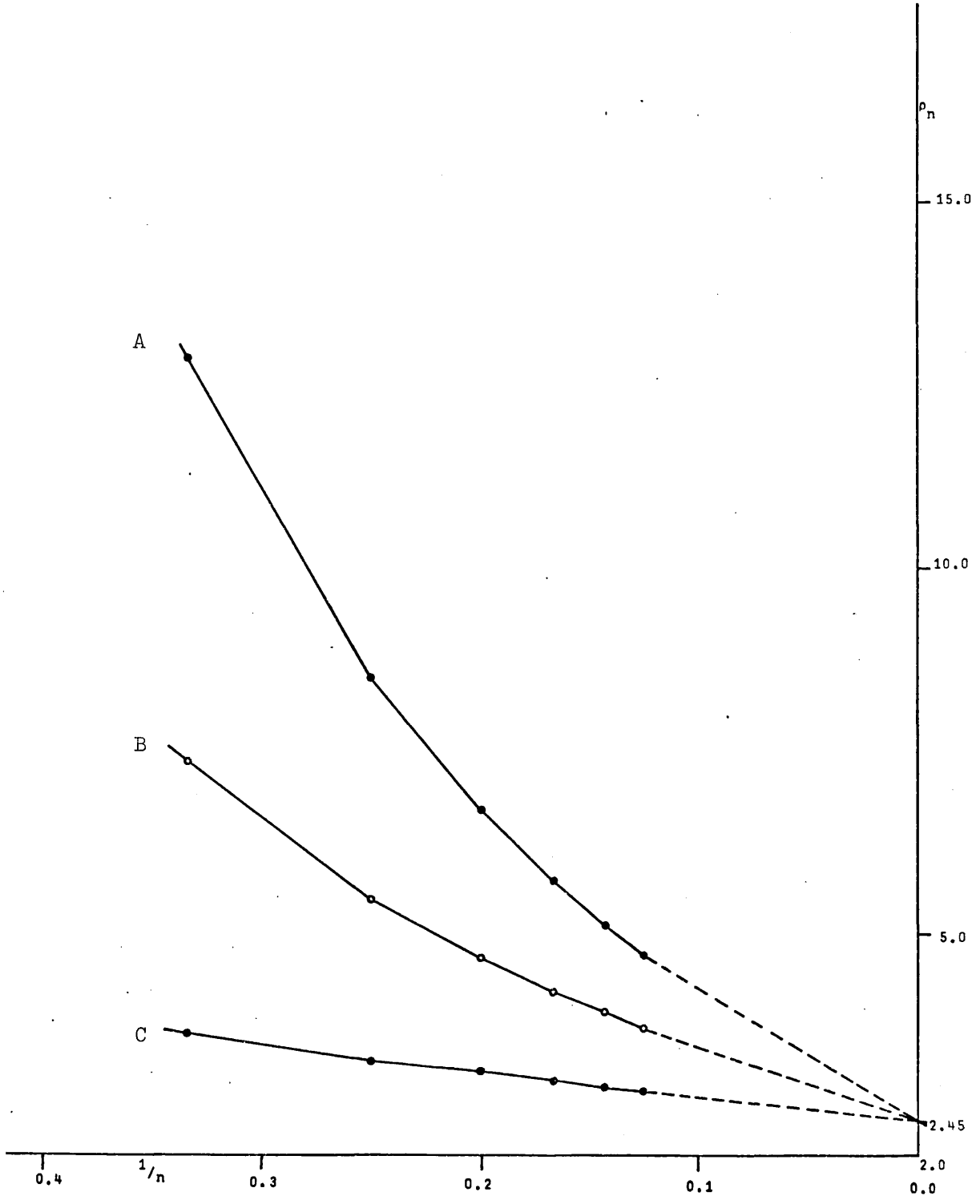


Fig. 3.4 Simple Quadratic Matching Lattice site problem. Successive estimates for the critical percolation probability ($\rho_n \to 1/p_c$) plotted against 1/n . (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

Table 3.6

Successive estimates of $j(a_n)$, $j(b_n)$ and $j(c_n)$ using the above value of p_c

n	$j_n(a_n)$	$j_n(b_n)$	$j_n(c_n)$
3	1.4973	6.0361	12.7735
4	1.3819	4.9636	9.8834
5	1.4151	4.5744	8.6753
6	1.4001	4.3828	8.0518
7	1.3897	4.2638	7.6733
8	1.4138	4.1968	7.4287

From the above estimates graphs of j_n against $1/n$ were plotted, Fig. 3.5, and this leads us to estimations of j as

$$j(a_n) = 1.4 \pm 0.1$$

$$j(b_n) = 3.8 \pm 0.1$$

$$j(c_n) = 6.2 \pm 0.1 \quad .$$

This would indicate a gap index Δ of 2.4 ± 0.2 and a value for g as $3 - \frac{2.4 \pm 0.1}{2.4 \pm 0.2}$.

Again with the restriction that $g \geq 2$ we may reduce the error limits on Δ to

$$\Delta = 2.4 \begin{matrix} + 0.2 \\ - 0.1 \end{matrix}$$

and

$$g = 2.0 + 0.12 \quad .$$

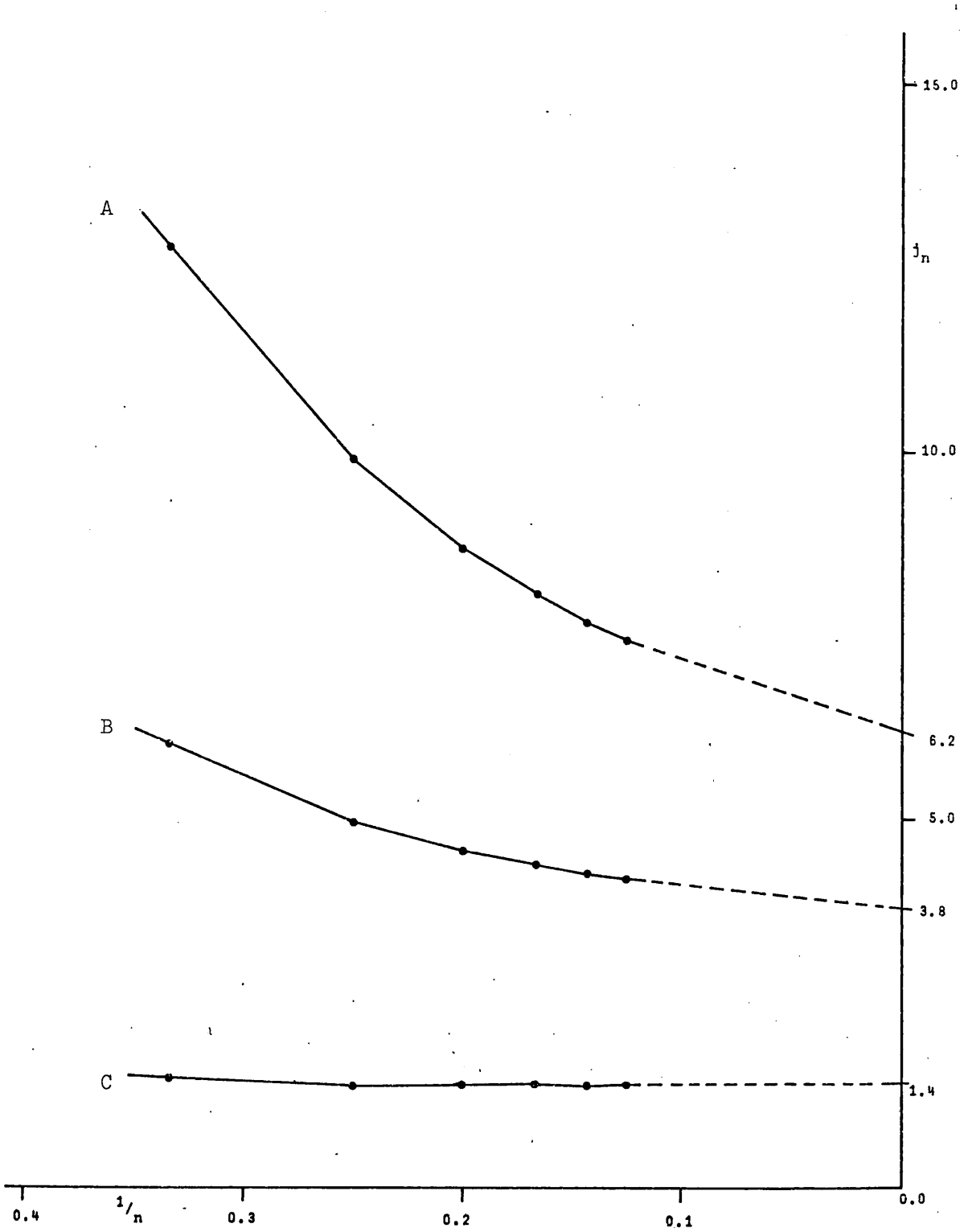


Fig. 3.5 Simple Quadratic Matching Lattice site problem. Successive estimates j_n for the index of the different moment expansions plotted against $1/n$. (A) Fourth moment expansion(B) Third moment expansion (C) Mean size expansion.

3.4 Triangular Lattice - Site Problem

It is important to study this lattice since the exact value of p_c is known. This allows us to obtain a measure of the accuracy of series expansion techniques.

Table 3.7

Coefficients for expansion of $S(p)$, $M_3(p)$ and $M_4(p)$. We quote the successive coefficients in tabular form.

n	a_n	b_n	c_n
1	6	18	42
2	18	120	522
3	48	552	3840
4	126	2160	21654
5	300	7428	101964
6	750	24162	429762
7	1686	72882	1649226
8	4074	214248	5947098
9	8868	598464	20231460

The exact value of $p_c = \frac{1}{2}$.

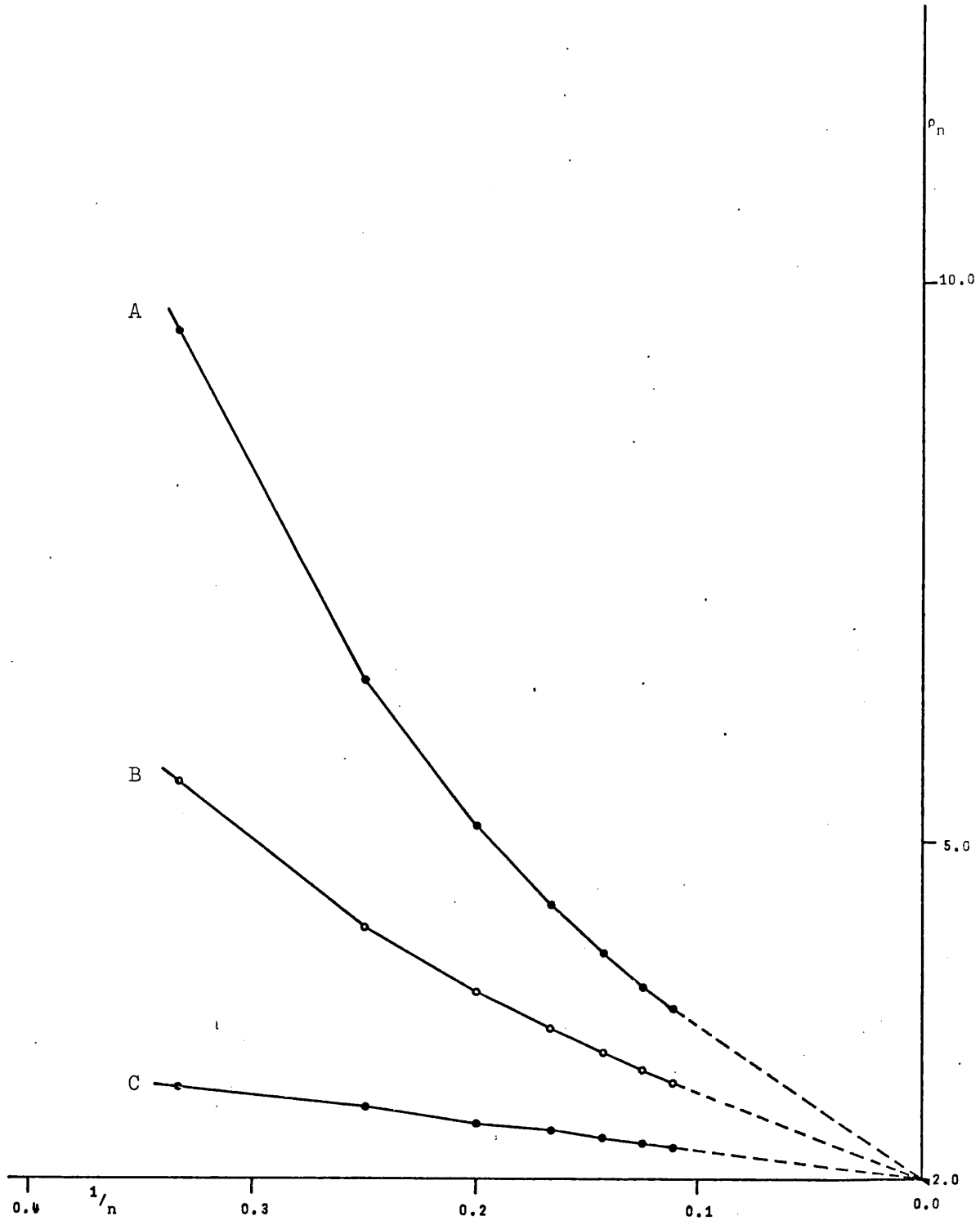


Fig. 3.6 Triangular Lattice site problem. Successive estimates for the percolation probability ($\rho_n \to 1/p_c$) plotted against 1/n . (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

Table 3.8

Ratios of coefficients of $\rho_n(a_n)$, $\rho_n(b_n)$ and $\rho_n(c_n)$

n	$\rho_n(a_n)$	$\rho_n(b_n)$	$\rho_n(c_n)$
3	2.8284	5.5377	9.5618
4	2.6458	4.2426	6.4407
5	2.5000	3.6683	5.1530
6	2.4398	3.3446	4.4550
7	2.3707	3.1324	4.0218
8	2.3307	2.9778	3.7200
9	2.2934	2.8656	3.5025

The exact value of p_c is 0.5 and Fig. 3.6 can be seen to be converging to this value fairly rapidly.

Table 3.9

Successive estimates of $j(a_n)$, $j(b_n)$ and $j(c_n)$ for $p_c = 0.5$.

n	$j_n(a_n)$	$j_n(b_n)$	$j_n(c_n)$
3	1.2426	5.3066	11.3427
4	1.2915	4.4853	8.8814
5	1.2500	4.1708	7.8824
6	1.3193	4.0337	7.3649
7	1.2973	3.9633	7.0762
8	1.3227	3.9111	6.8798
9	1.3204	3.8950	6.7611

From Fig. 3·7 the convergence of the j_n 's is seen to be relatively slow, but the data is consistent with the assumption

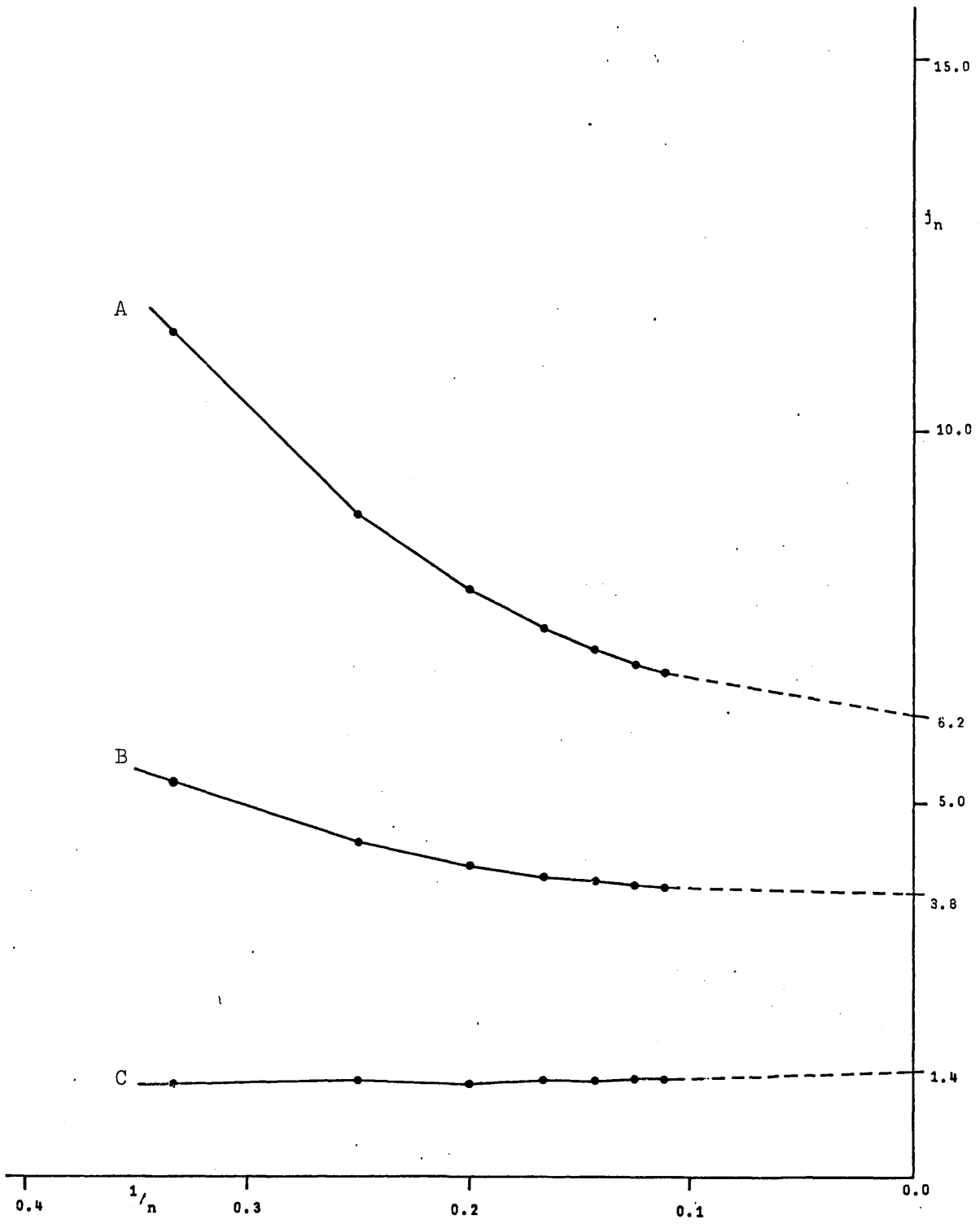


Fig. 3.7 Triangular Lattice site problem. Successive estimates j_n for the index of the different moment expansions plotted against $1/n$. (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

that they have the same limits as the two previous lattices.

Namely

$$j(a_n) = 1.4$$

$$j(b_n) = 3.8$$

$$j(c_n) = 6.2 \quad .$$

Giving a gap index, as before, of 2.4.

3.5 Face Centred Cubic Lattice - Site Problem

Table 3.10

Coefficients for expansion of $S(p)$, $M_3(p)$ and $M_4(p)$ we quote the successive coefficients in tabular form

n	a_n	b_n	c_n
1	12	36	84
2	84	552	2388
3	504	5880	41136
4	3012	53280	544668
5	17142	433362	6095418
6	96228	3280224	60712596
7	532028	23558748	555088244

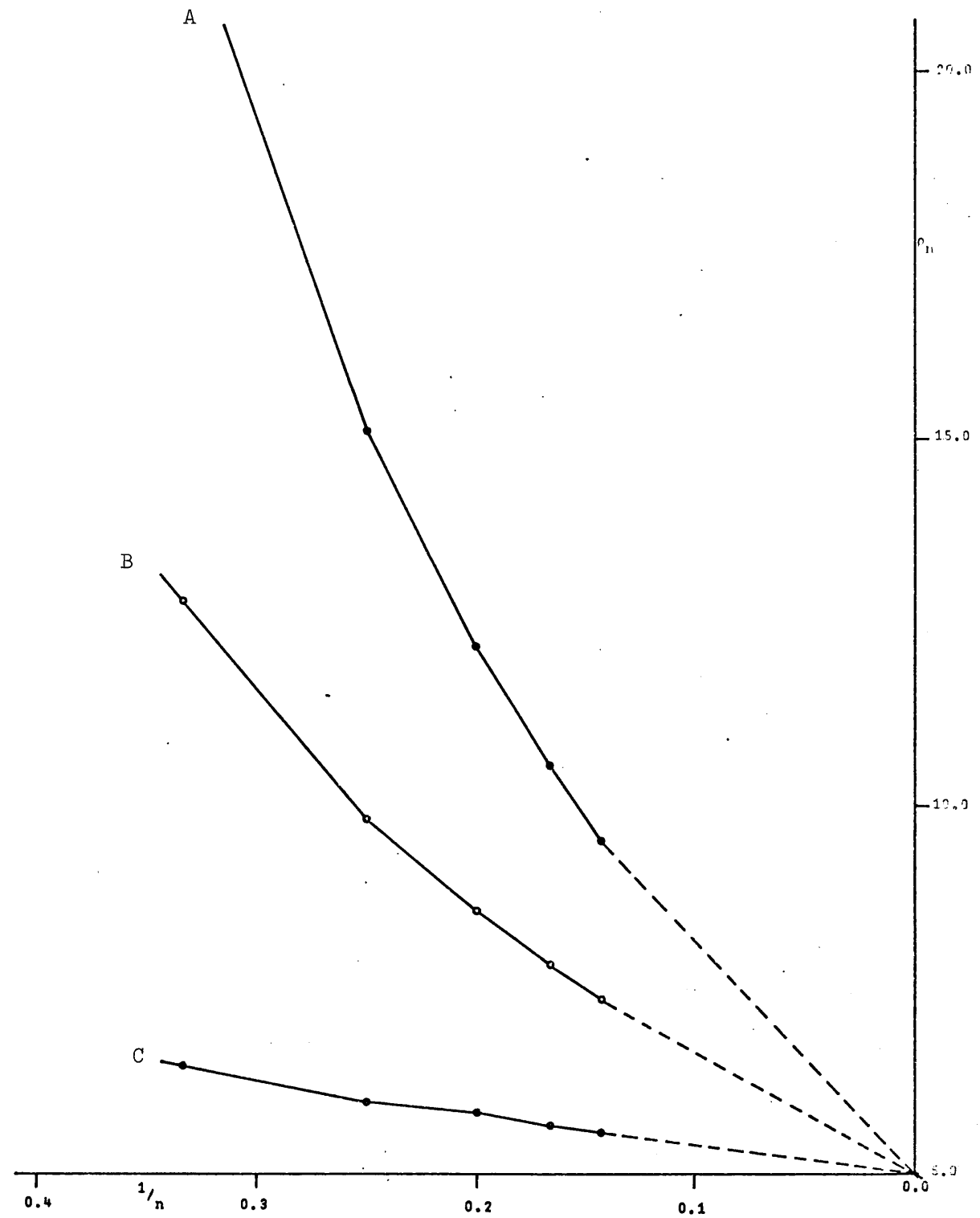


Fig. 3.8 . Face Centred Cubic Lattice site problem. Successive estimates for the critical percolation probability ($\rho_n \to 1/p_c$) plotted against 1/n . (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

Table 3.11

Ratios of coefficients $\rho_n(a_n)$, $\rho_n(b_n)$ and $\rho_n(c_n)$

n	$\rho_n(a_n)$	$\rho_n(b_n)$	$\rho_n(c_n)$
2	9.1652	23.4947	48.8672
3	6.4807	12.7802	22.1295
4	5.9881	9.8245	15.1025
5	5.8320	8.5849	12.1728
6	5.6523	7.8464	10.5578
7	5.5710	7.3731	9.5429

From Fig. 3.8 the estimated value for p_c on this lattice is

$$p_c = 0.198 \pm 0.002 \quad .$$

Table 3.12

Successive estimates of $j(a_n)$, $j(b_n)$ and $j(c_n)$ using the above value of p_c

n	$j_n(a_n)$	$j_n(b_n)$	$j_n(c_n)$
3	0.8496	4.5914	10.1449
4	0.7426	3.7811	7.9612
5	0.7737	3.4991	7.0511
6	0.7149	3.3215	6.5427
7	0.7215	3.2191	6.2264

From the above information estimates of j were made, see Fig. 3.9, these were

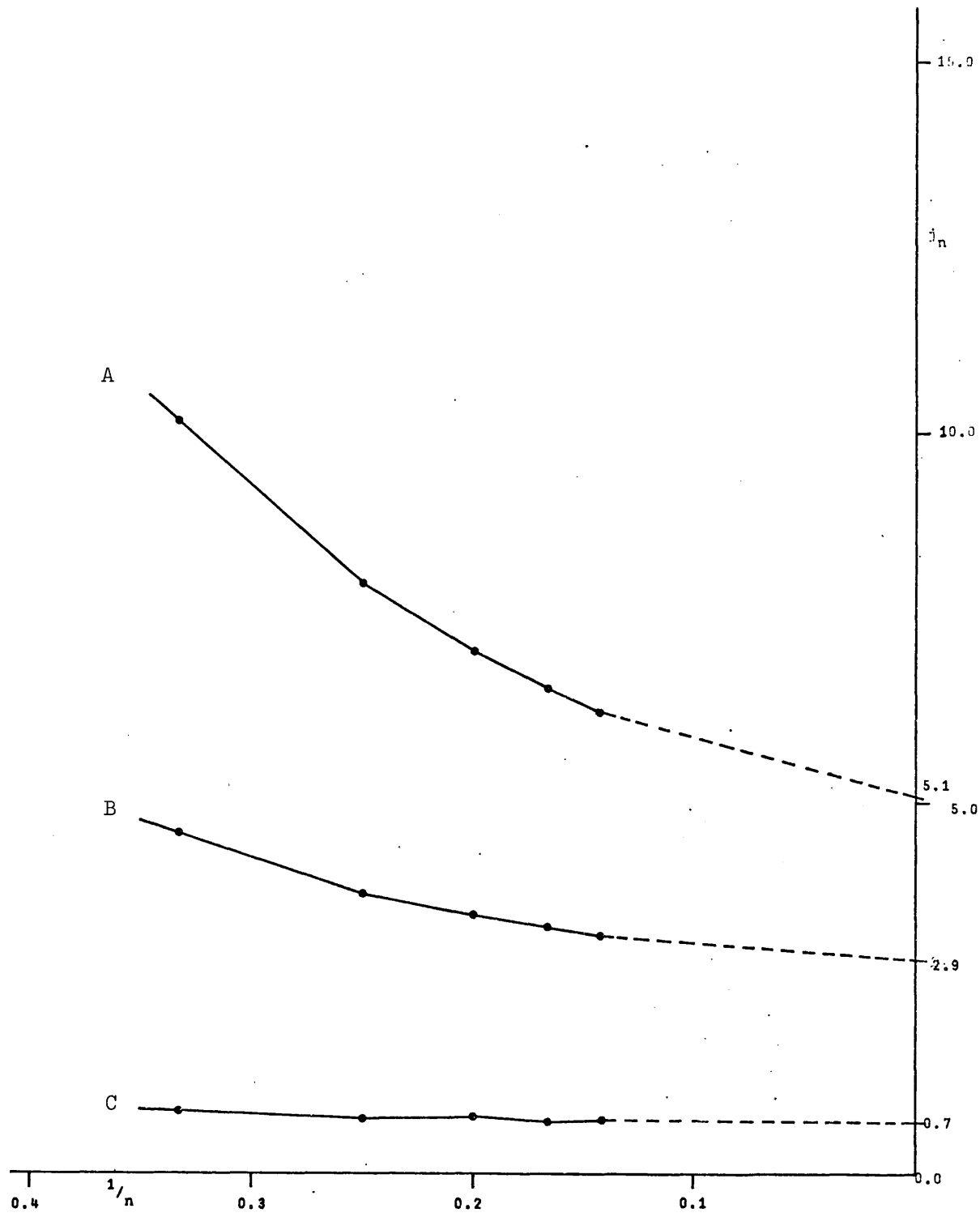


Fig. 3.9 Face Centred Cubic Lattice site problem. Successive estimates j_n for the index of the different moment expansions plotted against $1/n$. (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

$$j(a_n) = 0.70 \pm 0.02$$

$$j(b_n) = 2.9 \pm 0.1$$

$$j(c_n) = 5.1 \pm 0.1 \quad .$$

This would give, for three dimensions, an estimated value for the gap index Δ of 2.2 ± 0.2. Hence we obtain $g = 2.23 \pm 0.08$.

3.6 Face Centred Cubic Lattice - Bond Problem

Table 3.13

Coefficients for expansion of $S(p)$, $M_3(p)$, and $M_4(p)$ we quote the successive coefficients in tabular form.

n	a_n	b_n	c_n
1	22	66	154
2	234	1632	7218
3	2348	28524	204908
4	22726	422592	4459822
5	214642	5660238	82265926
6	1993002	70767942	1354071174
7	18266276	841184856	20495769944
8	165690848	9616920970	290829802076

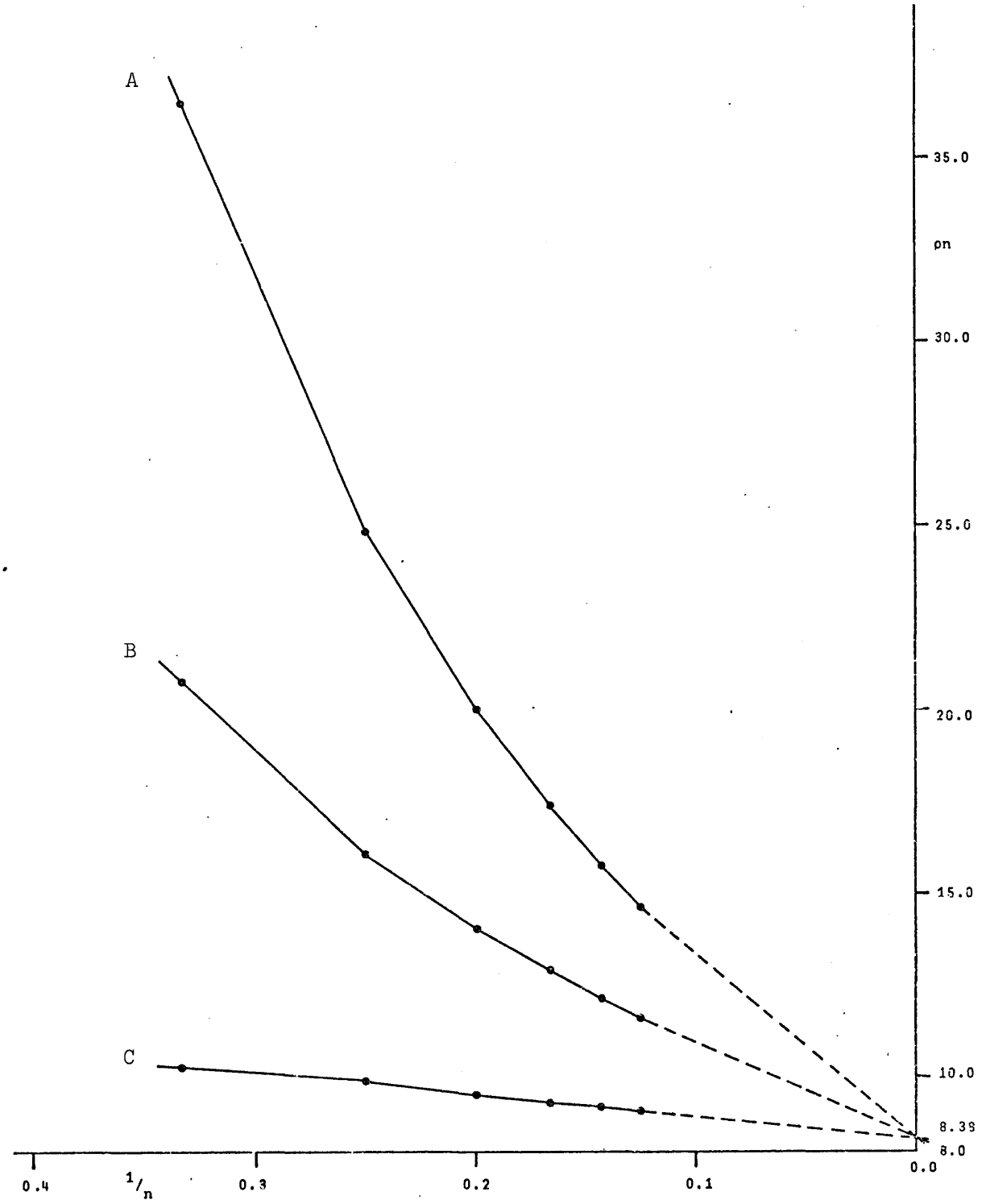


Fig. 3.10 Face Centred Cubic Lattice bond problem. Successive estimates for the critical percolation probability ($\rho_n \to 1/p_c$) plotted against $1/n$. (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

Table 3.14

Ratios of coefficients $\rho_n(a_n)$, $\rho_n(b_n)$ and $\rho_n(c_n)$

n	$\rho_n(a_n)$	$\rho_n(b_n)$	$\rho_n(c_n)$
3	10.3309	20.7890	36.4770
4	9.8549	16.0916	24.8571
5	9.5611	14.0868	20.0369
6	9.3647	12.9407	17.4246
7	9.2250	12.1907	15.7842
8	9.1179	11.6573	14.6554

From extrapolations based on table 3.14 the estimated value for p_c , see Fig. 3.10, is $p_c = 0.1193 \pm 0.0002$.

Table 3.15

Successive estimates of $j(a_n)$, $j(b_n)$ and $j(c_n)$ using the above value of p_c

n	$j(a_n)$	$j(b_n)$	$j(c_n)$
3	0.6974	4.4404	10.0551
4	0.7028	3.6789	7.8618
5	0.7032	3.4028	6.9520
6	0.7032	3.2630	6.4725
7	0.7038	3.1804	6.1814
8	0.7021	3.1258	5.9871

From the above information estimates of j were made using a Nevilles Table, see Fig. 3.11, these were

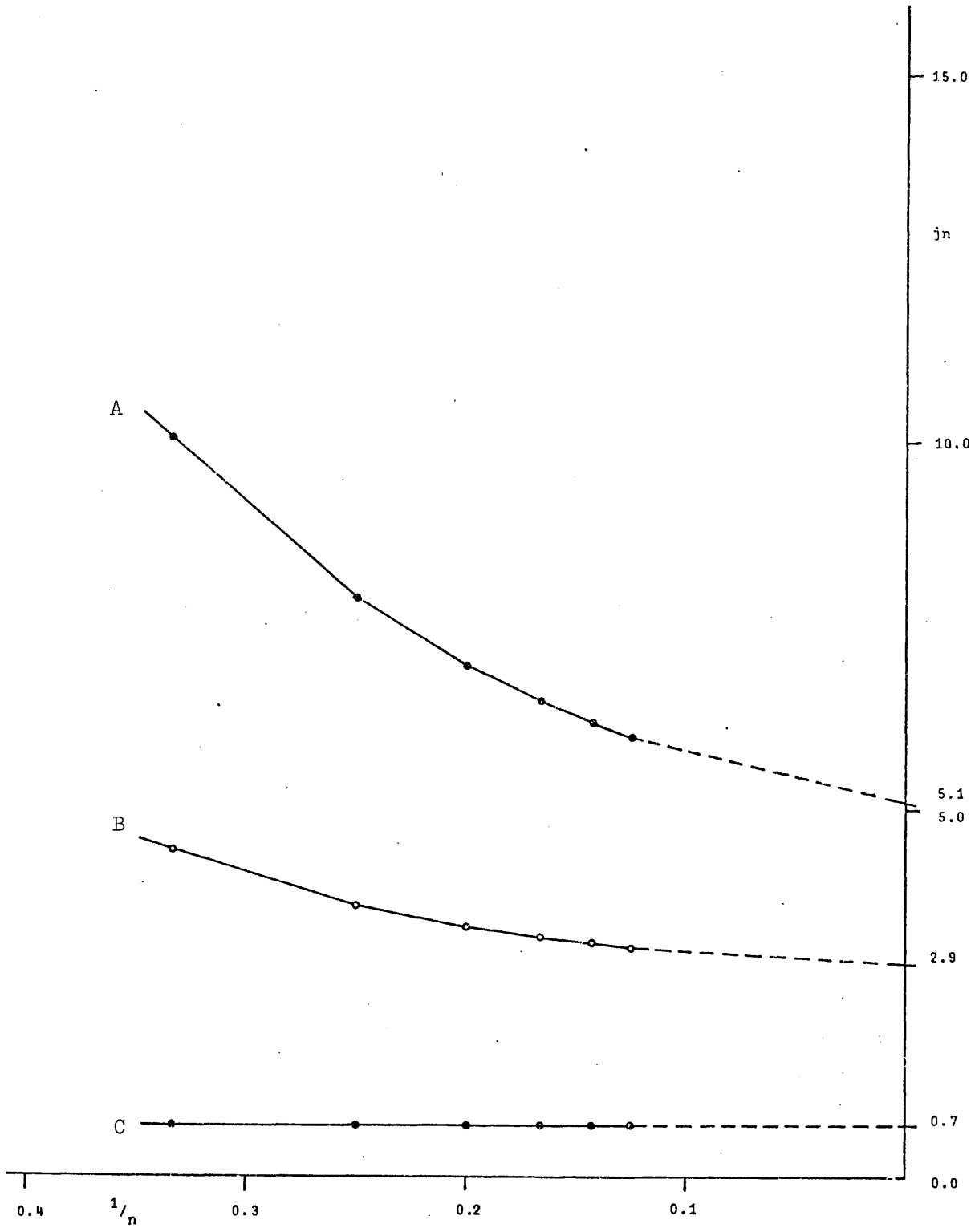


Fig. 3.11 Face Centred Cubic Lattice bond problem. Successive estimates j_n for the index of different moment expansions plotted against $1/n$. (A) Fourth moment expansion (B) Third moment expansion (C) Mean size expansion.

$$j(a_n) = 0.70 \pm 0.01$$

$$j(b_n) = 2.9 \pm 0.1$$

$$j(c_n) = 5.1 \pm 0.1 \quad .$$

These results are consistent with those derived for the F.C.C. lattice site problem and give the same results for both Δ and g .

3.7 Estimates of γ , Δ and g from series extrapolation techniques

From the previous sections it would seem reasonable to suppose that the n^{th} moment of the cluster size distribution varies as

$$M_n(p) \sim (p_c - p)^{-\gamma-(n-2)\Delta}$$

where in two dimensions

$$\gamma = 2.40 \pm 0.1$$

$$\Delta = 2.40 \pm 0.2$$

$$g = 2.0 + 0.1 \quad .$$

For three dimensions

$$\gamma = 1.70 \pm 0.02$$

$$\Delta = 2.25 \pm 0.25$$

$$g = 2.24 \pm 0.09 \quad .$$

Once we have decided upon a value for j we can estimate the radius of convergence of the series, see [21], by calculating

$$\beta_n = (n+j)/n\rho_n \quad .$$

The quantity β_n should converge to p_c with almost negligible slope. Even if the estimate for j is incorrect β_n must still converge to p_c. In Table 3.16 we list β_n for the site problem on the triangular, simple quadratic matching and honeycomb matching lattices. In Table 3.17 β_n is quoted for the F.C.C. site problem and the F.C.C. bond problem.

Table 3.16

Site problem: Two dimensional lattices: successive estimates for the critical probability $\beta_n = (n+j)/n\rho_n$ $\quad j = 1.4$

n	Triangular	Simple Quadratic Matching Lattice	Honeycomb Matching Lattice
4	0.5103	0.4094	0.2965
5	0.5120	0.4070	0.2999
6	0.5055	0.4080	0.3006
7	0.5062	0.4085	0.3011
8	0.5041	0.4074	0.3014
9	0.5039		
Estimated value of p_c	0.5 Exact	0.408 ± 0.002	0.302 ± 0.002

Table 3.17

Three dimensional lattices: successive estimates for the critical probability $\beta_n = (n+j)/np_n$ $j = 0.7$

n	Face Centred Cubic Lattice Site Problem	Face Centred Cubic Lattice Bond Problem
4	0.19622	0.11922
5	0.19547	0.11923
6	0.19756	0.11924
7	0.19744	0.11924
8		0.11927
Estimated value of p_c	0.198 ± 0.001	0.1193 ± 0.0001

3.8 Derivation of an Upper Bound for a Random Plane Network [5]

To construct a random plane network first pick points from the infinite plane by a Poisson process, with density D points per unit area. Next join each pair of points by a line if they are separated by a distance less than R.

Gilbert shows [5] that in two dimensions a lower bound for E_c is 1.75 where $E = \pi R^2 D$ and E_c is the value of E such that

$$\lim_{N\to\infty} P(N) = P(\infty) \neq 0$$

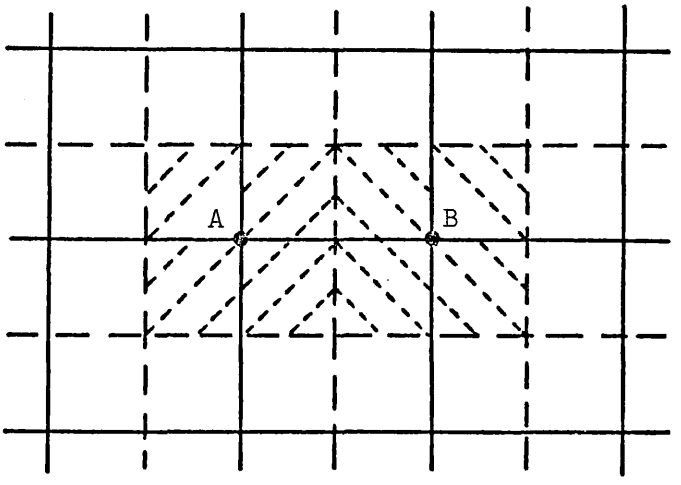
where $P(N)$ is the probability that a point belongs to a component containing at least $N-1$ points.

Gilbert points out that a correspondence between percolation processes and the random plane network can supply an upper bound for E_c . He obtains a value 17.4 for this bound. To reduce this bound it is necessary to increase the similarity between the two processes. To do this we wish to make the distance R in the random plane as near to the nearest neighbour distance on the lattice as possible.

Consider the case of the simple quadratic lattice (bond problem) and separate the bonds as shown in Fig. (3.12).

We say that if any two points are connected in the squares A and B then the bond AB is occupied.

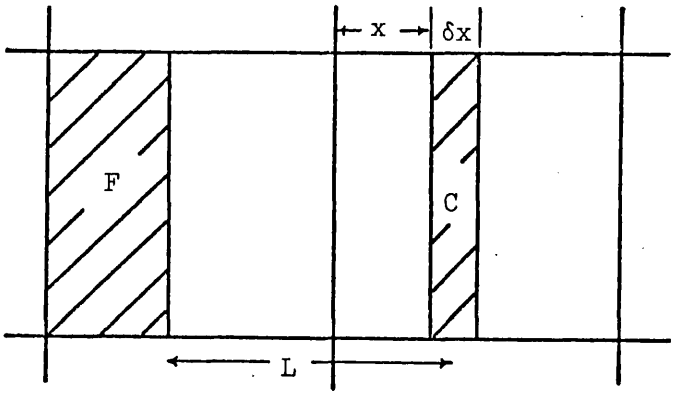
Fig. 3.12



The probability that a point in C is connected to a point in F , see Fig. (3.13), is

$$dp = (1 - e^{-DL(L-x)})(1 - e^{-DL\delta x}) \quad .$$

Fig. 3.13



Hence the total probability that the bond AB is occupied is

$$p = \int_o^L (1 - e^{-DL(L-x)})DLdx$$

$$= DL^2 + e^{-DL^2} - 1$$

$$p = \frac{EL^2}{\pi R^2} + e^{-\frac{EL^2}{\pi R^2}} - 1 \qquad (3.14)$$

Now we need to choose R to be the length of the diagonal of the square since we wish to be able to say that any two points in the square are connected. This ensures that if two bonds are connected in the lattice case then there is at least one path between them in the random plane case, thus providing an upper bound.

The selection of R as the diagonal rather than the side of the square does not affect the argument since increasing R

increases the upper bound. Substituting $R^2 = 2L^2$ in (3.14) gives

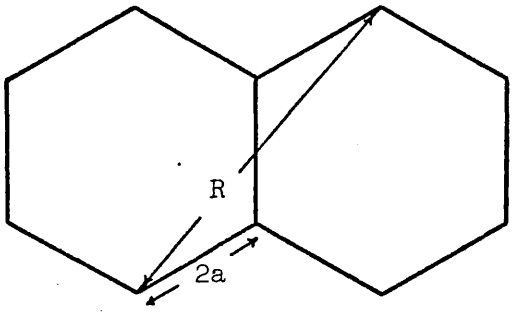
$$p = \frac{E}{2\pi} + e^{-E/2\pi} - 1 \quad . \tag{3.15}$$

For the simple quadratic bond problem we know that $p_c = \frac{1}{2}$ hence a bound for E_c can be calculated.

$$E_c \leq 7.6 \ .$$

For the triangular lattice bond problem we must consider hexagonal areas, see Fig. (3.14).

Fig. 3.14



Using the same method as that described above we see that

$$p = \frac{6\sqrt{3}a^2E}{\pi R^2} + \exp\left(-\frac{6\sqrt{3}a^2E}{\pi R^2}\right) - 1$$

$R = 28a^2$ hence

$$1 + p = \frac{3\sqrt{3}E}{14\pi} + \exp(-\frac{3\sqrt{3}E}{14\pi}) \quad . \tag{3.16}$$

For this lattice $p_c = 0.347296$ and we obtain for E_c

$$E_c \leq 9.0 \quad .$$

Since the first lattice supplies a better upper bound we choose that value and finally obtain as bounds for E_c

$$1.75 \leq E_c \leq 7.6 \quad .$$

Chapter 4 The Scaling Laws for Percolation Processes [29]

4.1 Analogy between the mean number of clusters and the free energy of a ferromagnet

So far we have endeavoured to derive estimates for the critical exponents on various lattices. We have shown for the Bethe lattice that the indices for the n^{th} moment cluster size differ by a constant Δ and indicated the truth of this statement for various two and three dimensional lattices. We wish now to derive the scaling laws which describe the behaviour near the critical point. These are then tested using the exact solution for the Bethe lattice and the numerical work of chapter 3 is found to be consistent with the scaling hypothesis.

An analogy between percolation and ferromagnetism has been drawn by Kasteleyn and Fortuin [30], namely

mean number of clusters $\leftrightarrow$ free energy

percolation probability $\leftrightarrow$ spontaneous organisation

mean size of finite clusters $\leftrightarrow$ initial susceptibility .

The basis for this analogy may be seen by considering the moment generating function for the site (bond) problem

$$k(p,\lambda) = \sum_s \langle n_s \rangle \lambda^s \quad . \tag{4.10}$$

The mean number of clusters of size s, $\langle n_s \rangle$ is calculated per site (bond) of the lattice, the lattice being assumed infinite

but only finite clusters being counted. Clearly $k(p,1)$ is the mean number of finite clusters of any size or briefly the mean number of clusters. The parameter λ will be treated as analogous to the magnetic field parameter $\exp(-\frac{2mH}{K_B T})$ so that $\lambda = 1$ corresponds to zero field and $k(p,\lambda)$ is then analogous to the free energy in a magnetic field. The temperature analogue is the probability p and

$$p < p_c \Leftrightarrow T > T_c$$

$$p > p_c \Leftrightarrow T < T_c$$

where p_c is the probability above which infinite clusters are to be found.

The field derivatives of the free energy correspond to the moments

$$m_j(p) = \left(\lambda \frac{\partial}{\partial\lambda}\right)^j k(p,\lambda)\Big|_{\lambda=1}$$

$$= \sum_s s^j \langle n_s \rangle \quad . \tag{4.11}$$

The first moment is the mean number of particles per site (bond) which belong to finite clusters, or p times the probability that the particle is contained in a finite cluster. The percolation probability is defined as the probability that the particle belongs to an infinite cluster thus

$$P(p) = 1 - p^{-1} m_1(p) \quad . \tag{4.12}$$

This function is the spontaneous magnetisation analogue being related to the first derivative of the mean number. It is zero below p_c just as the magnetisation vanishes above T_c. The second moment is the mean size of finite clusters which should therefore be taken as the susceptibility analogue. The mean size diverges in the limit $|p-p_c| \to 0$ just as the susceptibility diverges as $|T-T_c| \to 0$.

By numerical analysis of series expansions it was found, [31] and [32], that for the Ising model the j^{th} field derivative of the free energy in the limit $H \to 0$ is consistent with the asymtotic form

$$f_j(T) \sim |T-T_c|^{-\gamma-(j-2)\Delta} \tag{4.13}$$

where the exponents γ and Δ are approximately equal above and below T_c. This leads [33] to the scaling law for the singular part of the free energy

$$f_{sing.}(T,H) = |T-T_c|^{-\gamma+2\Delta} F\left(\frac{H}{|T-T_c|^{\Delta}}\right) \tag{4.14}$$

we now wish to propose a similar result for percolation processes the form of which is clear from the analogy. The proposal will be supported by the exact analysis on the Bethe lattice and by numerical work.

4.2 The Scaling Laws for Percolation Processes

In their analysis of the Bethe lattice, Fisher and Essam [25] used the generating function

$$K(x,y) = \sum_{s,t} k_{st} x^s y^t \quad . \tag{4.15}$$

We shall make use of the relation

$$k(p,\lambda) = K(p\lambda, 1-p) \tag{4.16}$$

on comparison with equation (4.10)

$$\langle n_s \rangle = \sum_{t} k_{st} p^s (1-p)^t \quad . \tag{4.17}$$

On the Bethe lattice, the perimeter is uniquely related to size so that in this case there is only one term in the sum, but equation (4.17) is a result which may be applied to any lattice. This unique relation of perimeter to size enabled an exact expression for k_{st} to be found from which we deduce

$$k_{st} \underset{s\to\infty}{\sim} s^{-g} \nu^s \tag{4.18}$$

where in terms of the coordination number $\sigma + 1$,

$$\nu = \sigma^\sigma/(\sigma-1)^{\sigma-1} \qquad \text{and} \qquad g = 5/2$$

this result together with

$$t = (\sigma-1)s + t_o(\sigma)$$

gives

$$\langle n_s \rangle \equiv k_{st} p^s (1-p)^t$$

$$\underset{s\to\infty}{\sim} s^{-g}\{\mu(p)\}^s \qquad (4.19)$$

where

$$\mu(p) = \nu p(1-p)^{\sigma-1} \qquad (4.20)$$

and hence in the limit $\lambda\mu(p) \to 1$ from below, we have

$$k_{sing}(p,\lambda) \sim \{1 - \lambda\mu(p)\}^{g-1} \quad . \qquad (4.21)$$

When $\lambda = 1$ equation (4.21) implies that there is a singularity in the mean number at $p = p_c$,

where

$$\mu(p_c) = 1 \quad .$$

Thus

$$p_c(1-p_c)^{\sigma-1} = \frac{1}{\nu} = \frac{1}{\sigma}(1 - \frac{1}{\sigma})^{\sigma-1} \qquad (4.22)$$

and there is just one solution in the interval $(0,1)$, namely

$$p_c = \frac{1}{\sigma}$$

since $\mu(p)$ also has its maximum value at p_c . Expanding $\mu(p)$ around p_c

$$\mu(p) \sim 1 - A|p-p_c|^{\Delta} \qquad (4.23)$$

where for the Bethe lattice $\Delta = 2$ and $A = \sigma^3/2(\sigma-1)$. The function $k_{sing.}(p,\lambda)$ has no singularities for $\lambda < 1$ (cf. the Yang and Lee theorem for the Ising Model). For given p there is a singularity at

$$\lambda = \lambda_c(p) = \frac{1}{\mu(p)} \geq 1 \quad . \tag{4.24}$$

This critical curve corresponds to the 'pseudo' spinodal curve for the Ising Model, [34]. Substituting equation (4.23) into (4.21) we obtain

$$k_{sing}(p,\lambda) \sim \{1 - \lambda(1 - A|p-p_c|^{\Delta})\}^{g-1} \quad . \tag{4.25}$$

By differentiating this j times with respect to λ we further obtain

$$m_j(p) \sim B_j|p-p_c|^{(g-1-j)\Delta} \tag{4.26}$$

where

$$B_j = (1-g)(2-g) \ldots\ldots(j-g)A^{g-1-j} \quad .$$

Equation (4.26) is analogous to (4.13) and by comparison

$$\gamma = (3 - g)\Delta$$

a result we obtained in Chapter 1, which gives $\gamma = 1$ for the Bethe lattice corresponding to a simple pole in the mean size at $p = p_c$. The result which corresponds to (4.14) may be obtained by writing $\lambda = \exp(-\xi)$, thus

$$k_{sing}(p,\lambda) \sim |p-p_c|^{-\gamma+2\Delta} G\left(\frac{\xi}{|p-p_c|^{\Delta}}\right) \quad .$$

The critical exponents are restricted by the exact result that $P(p)$ is finite. From equations (4.26) and (4.12)

$$P(p) \sim (p-p_c)^{\Delta-\gamma}$$

for

$$p \to p_c^+$$

and hence $\Delta \geq \gamma$.

An obvious extension of $P(p)$ to finite $\lambda < 1$ and use of equation (4.21) yields

$$P(p_c,\lambda) \sim (1 - \lambda)^{g-2}$$

for $\lambda \to 1^-$

and hence $g \geq 2$ a result used in Chapter 3 to confine the error bounds on g .

Numerical work on series expansions for various two and three dimensional lattices supports the conjecture that equations (4.21), (4.23), (4.25) and (4.26) are generally valid but with different values of the two independant exponents γ and Δ . The results indicating the validity of (4.26) for $j = 2$, 3 and 4 are listed in Chapter 3.

To test the validity of (4.23) plots of $\langle n_{s+1} \rangle / \langle n_s \rangle$ were made for many values of p in the range

$$10^{-5} < \frac{|p-p_c|}{p_c} < 10^{-1}$$

now from (4.19)

$$\langle n_{s+1} \rangle / \langle n_s \rangle \sim \mu(p)(1 - g/s) \quad . \tag{4.27}$$

Hence if $\langle n_{s+1} \rangle / \langle n_s \rangle$ is plotted against $1/s$ the intercept should give a value for $\mu(p)$, and the gradient a value for g . The results which now follow were obtained using the cluster expansions of the face centred cubic lattice site problem. This lattice was chosen since the ratios $\langle n_{s+1} \rangle / \langle n_s \rangle$ seemed to converge smoothly to $\mu(p)$.

In order to estimate the correct intercept a Nevilles table was plotted from the ratio values. A sample of the computer output is listed in Table 4.1 for $p = 0.19346$. The number of decimal places used was however much greater than in the figures recorded.

The value which appeared in the last column of the Nevilles table was the one used for $\mu(p)$ for each value of p .

One expects the maximum value of $\mu(p) = 1$ to occur at $p = p_c$. The Nevilles table however did not give these results. The maximum value on the F.C.C. lattice occurred at $p = 0.19346$ instead of at the expected value of $p = 0.198$. The maximum value of $\mu(p)$ was also given as 1.00123180 .

One can see the reason for these apparent discrepancies when one considers how they were derived. The Neville Table

Table 4.1

Sample of the computer output to estimate $\mu(p)$ for a given value of p .

s	$\langle n_s \rangle$	$\frac{\langle n_{s+1} \rangle}{\langle n_s \rangle}$	Nevilles Table				
1	0.0146589						
2	0.0046838	0.3195					
3	0.0023769	0.5074	0.8834				
4	0.0014316	0.6023	0.8868	0.8902			
5	0.0009531	0.6658	0.9196	0.9688	1.0211		
6	0.0006785	0.7118	0.9422	0.9874	1.0061	0.9985	
7	0.0005067	0.7469	0.9570	0.9940	1.0029	1.0005	1.0012

values oscillate, albeit slightly, about the true result unless very many terms of the series are known. Another term in the series could have moved the maximum to a different position. By consistently chosing the last value in the Nevilles table we assume that this change in value of the variable will not change the shape of the $\mu(p)$ curve but rather only shift the axes.

In accordance with this assumption (4.23) was adjusted to give agreement with the Nevilles table results. The value of Δ should not be affected by this change.

Equation (4.23) them becomes

$$\mu(p) = M - A|p-p_m|^{\Delta} \qquad (4.28)$$

where

M is the maximum value of $\mu(p)$ and p_m is the value of p for which this occurs.

A graph of $\log[M - \mu(p)]$ plotted against $\log[|p-p_m|]$ should provide a value for Δ and A. The results were plotted over three decades for $p < p_m$ and $p > p_m$ and fitted extremely well onto two straight lines. In tables 4.2 and 4.3 the results are listed, Figs. 4.1 and 4.2 are the corresponding graphs.

Once it had been ascertained over which region the straight lines extended a least mean square fit was used on the points. This gave

$$\Delta = 2.0159 \qquad p < p_m$$

$$\Delta = 1.9856 \qquad p > p_m$$

$$\log(A) = 2.716 \qquad p < p_m$$

$$\log(A) = 2.502 \qquad p > p_m \quad .$$

The two results are extremely close together and we conclude that $\Delta = 2.0$ above and below p_c. This value is within error bounds of the value calculated in Chapter 3. Though if $\Delta = 2.0$ exactly this would mean that Δ does not change in going from the infinite (Bethe) lattice to three dimensions but then shows an appreciable jump in going to two dimensions.

Table 4.2

Selection of the values used, ranging over three decades, to plot Fig. 4.1 . $p < p_m$

p	$\mu(p)$	$-\log[\,\lvert p-p_m\rvert\,]$	$-\log[M-\mu(p)]$
0.19336	1.00123167	9.2103	15.8557
0.19334	1.00123161	9.0280	15.4762
0.19332	1.00123154	8.8739	15.1626
0.19308	1.00122986	7.8753	13.1528
0.19272	1.00122441	7.2089	11.8154
0.19236	1.00121544	6.8124	11.0207
0.19200	1.00120292	6.5293	10.4524
0.19164	1.00118684	6.3089	10.0097
0.18966	1.00103429	5.5728	8.5297
0.18606	1.00047309	4.9063	7.1839
0.18246	0.99953404	4.5099	6.3784
0.17886	0.99820309	4.2267	5.7996
0.17562	0.99646585	4.0063	5.3463

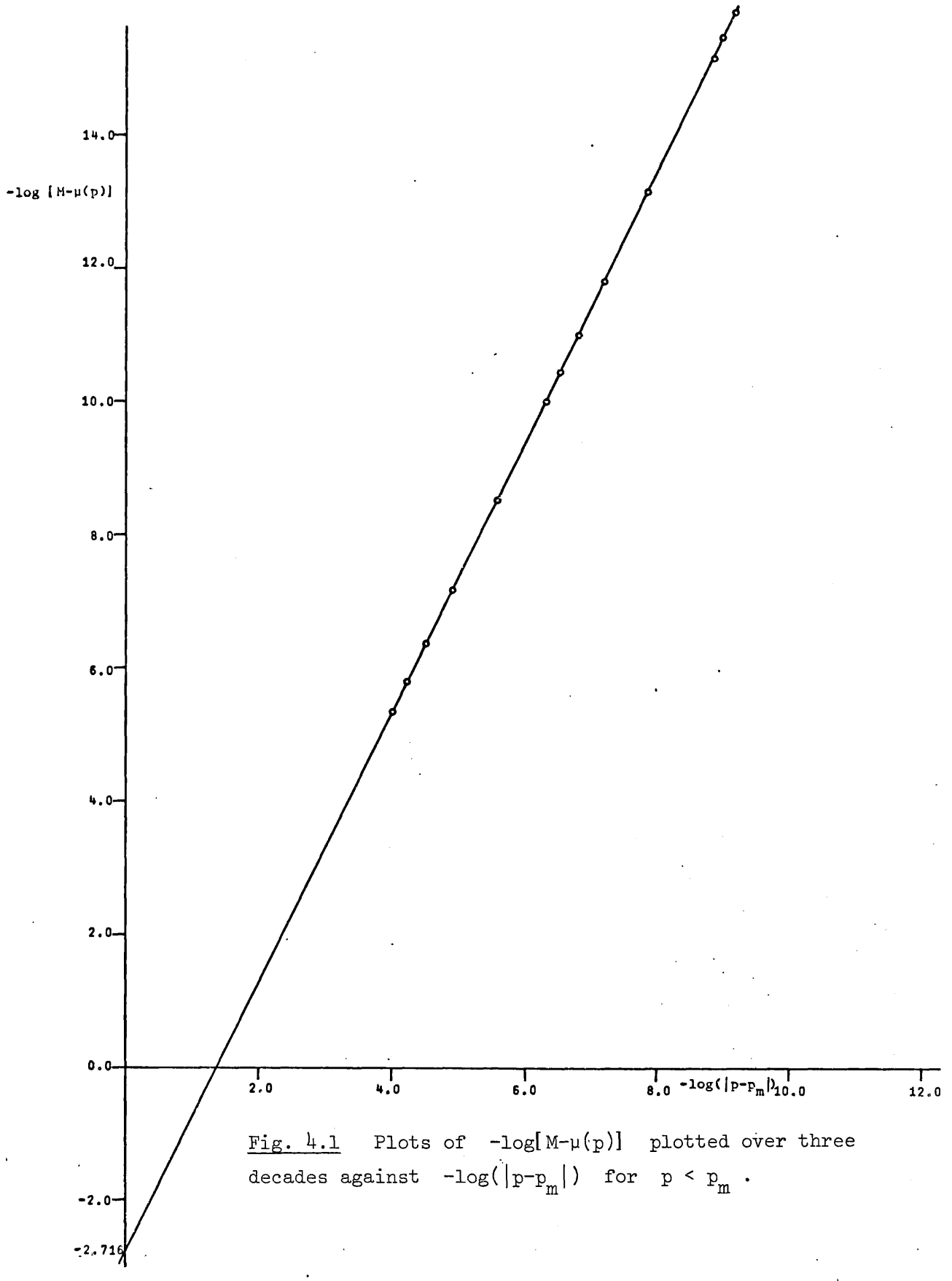


Fig. 4.1 Plots of $-\log[M-\mu(p)]$ plotted over three decades against $-\log(|p-p_m|)$ for $p < p_m$.

Table 4.3

Selection of values used, ranging over three decades, to plot Fig. 4.2 $p > p_m$

p	$\mu(p)$	$-\log[\,\lvert p-p_m\rvert\,]$	$-\log[M-\mu(p)]$
0.19354	1.00123171	9.4335	16.2235
0.19358	1.00123160	9.0280	15.4249
0.19362	1.00123145	8.7403	14.8653
0.19366	1.00123125	8.5172	14.4133
0.19386	1.00122962	7.8420	13.0362
0.19426	1.00122314	7.1309	11.6568
0.19466	1.00121237	6.7254	10.8487
0.19506	1.00119734	6.4378	10.2757
0.19546	1.00117804	6.2146	9.8310
0.19746	1.00101843	5.5215	8.4525
0.20146	1.00039032	4.8283	7.0803
0.20546	0.99936461	4.4228	6.2833
0.20946	0.99795786	4.1352	5.7218

In the above analysis we have assumed that the value of g is independant of p. To check this assumption the value of g was calculated for a large number of values of p using equation (4.27). The value of g would appear to vary very slowly with p but this may be because only a small number of terms are available. Over the range of p used the above assumption would appear to be valid.

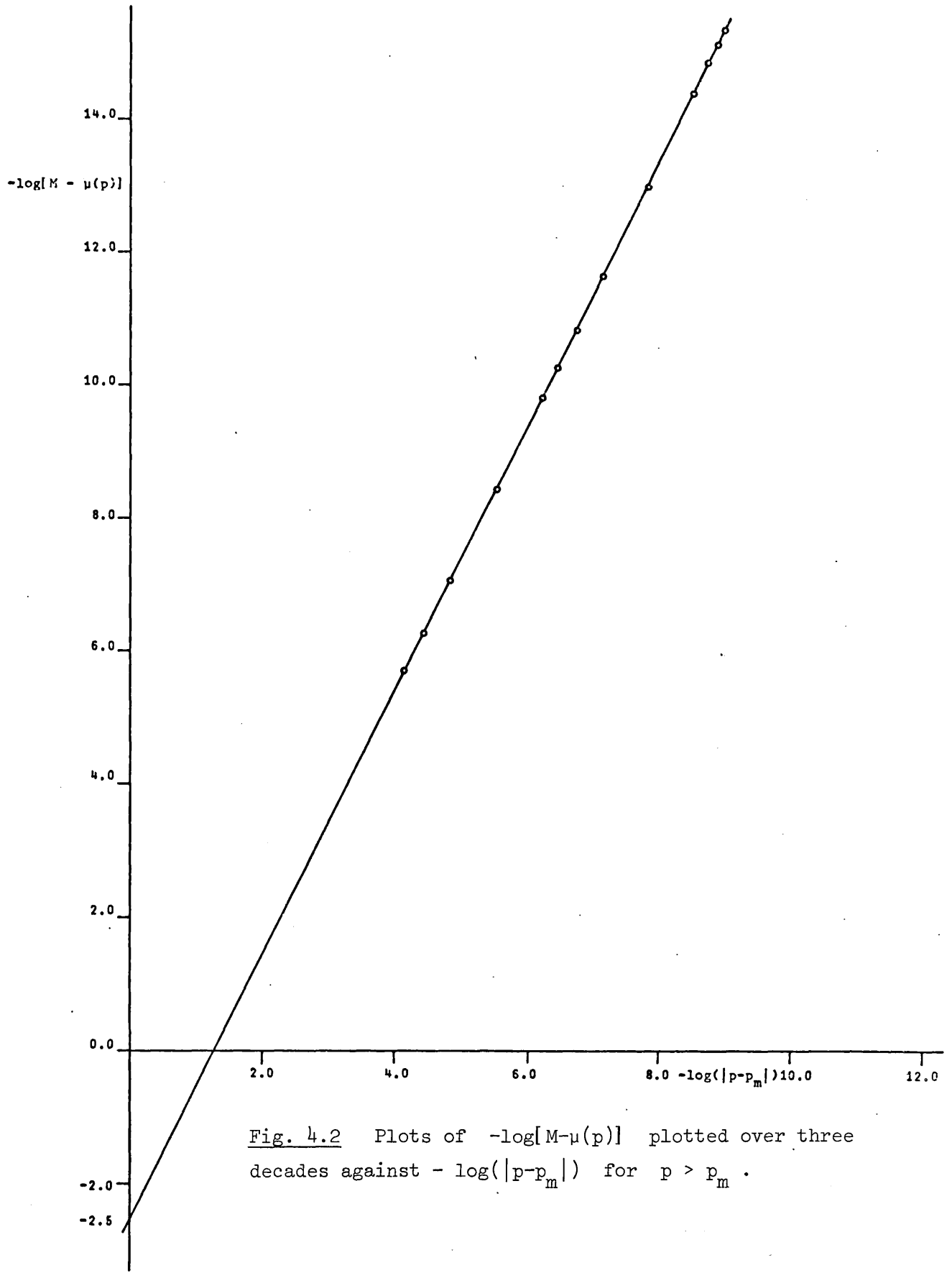


Fig. 4.2 Plots of $-\log[M-\mu(p)]$ plotted over three decades against $-\log(|p-p_m|)$ for $p > p_m$.

Chapter 5 Determination of the critical index δ at high and low temperatures for $p = 1$ and $p = p_c$

5.1 Calculation of δ for $p = p_c$ and $J >> k_B T$

It has been shown by Dr. J.W. Essam (on the Bethe lattice) using scaling arguments similar to those in the last chapter, that for $J >> k_B T$ and $p = p_c$ $M \sim H^{1/\delta}$. Where $1/\delta$ is related to g by the expression $1/\delta = g - 2$, therefore for the Bethe lattice $\delta = 2$.

We can show this directly in the following manner. We consider the bond problem with $J >> k_B T$. There will be a fixed number of atoms N and let there be n_t atoms in the t^{th} cluster then

$$M_t = m n_t \tanh \frac{m n_t H}{k_B T} \tag{5.10}$$

where M_t is the magnetisation of the t^{th} cluster.

$$M_t = m n_t \{ 1 - \frac{2\mu^{n_t}}{1+\mu^{n_t}} \} \tag{5.11}$$

where

$$\mu = e^{-\frac{2mH}{k_B T}} .$$

Now

$$M = \langle \Sigma_t M_t \rangle \tag{5.12}$$

hence

$$\frac{M}{N} = m\{1 - \frac{1}{N} \langle \Sigma_t \frac{2\mu^{n_t} n_t}{1 + \mu^{n_t}} \rangle \} . \tag{5.13}$$

If we consider the probability of a bond being occupied as p then

$$\frac{1}{N}\Big\langle \sum_t \frac{2n_t \mu^{n_t}}{1+\mu^{n_t}} \Big\rangle = 2\sum_r r b_r p^{r-1} q^{(\sigma-1)r+2} \frac{\mu^r}{1+\mu^r} \tag{5.14}$$

where $(\sigma-1)r+2$ is the perimeter of a cluster of r sites

b_r is the number of trees per site .

We digress at this point to consider the configurational generating function on the Bethe lattice.

$$K^s(x,y) = y^2 \sum_{r=1}^{\infty} b_r x^r y^{(\sigma-1)r} \quad . \tag{5.15}$$

Let

$$B_\sigma(Z) = \sum_{r=1}^{\infty} b_r Z^r \tag{5.16}$$

then

$$K^s(x,y) = y^2 B_\sigma(Z) \tag{5.17}$$

where

$$Z = xy^{\sigma-1} \quad .$$

Using arguments similar to those in Chapter 2, see [25], we can obtain $\frac{dB}{dZ}$ in the form

$$\frac{dB}{dZ} = [1 - X(Z)]^{-(\sigma+1)} \tag{5.18}$$

where $X(Z)$ is the root of $X(1-X)^{\sigma-1} = Z$ which vanishes with Z . For $\sigma = 2$ this can be easily solved and we obtain

$$\frac{dB}{dZ} = \frac{8}{\{1 + (1-4Z)^{\frac{1}{2}}\}^3} \quad . \tag{5.19}$$

From (5.16)

$$Z\frac{dB}{dZ} = \sum_{r=1}^{\infty} rb_r Z^r = \frac{8Z}{\{1 + (1-4Z)^{\frac{1}{2}}\}^3} \quad . \tag{5.20}$$

We can re-write (5.14) in the form

$$\frac{2q^2}{p} \sum_{n=1}^{\infty} (-1)^{n+1} \sum_{r=1}^{\infty} rb_r p^r q^{(\sigma-1)r} \mu^{nr} \quad . \tag{5.21}$$

Let $Z_n = pq^{\sigma-1}\mu^n$

then

$$\frac{2q^2}{p} \sum_{n=1}^{\infty} (-1)^{n+1} \sum_{r=1}^{\infty} rb_r p^r q^{(\sigma-1)r} \mu^{nr} = \frac{2q^2}{p} \sum_{n=1}^{\infty} (-1)^{n+1} \sum_{r=1}^{\infty} rb_r Z_n^r \quad . \tag{5.22}$$

Comparing the second sum on the right hand side of (5.22) with (5.20) we see that, for $\sigma = 2$

$$\frac{1}{N}\left\langle \Sigma_t \frac{2n_t \mu^{n_t}}{1 + \mu^{n_t}} \right\rangle = \frac{2q^2}{p} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{8Z_n}{\{1 + (1-4Z_n)^{\frac{1}{2}}\}^3}$$

$$= 16q^3 \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\mu^n}{\{1 + (1-4pq\mu^n)^{\frac{1}{2}}\}^3} \quad . \tag{5.23}$$

My thanks are due at this point to Dr. W.G. Chambers for introducing me to the Poisson summation formula by which the leading term of the above sum may be obtained in the following manner.

We write $\mu = e^{-C^*H}$ where $C^* = \frac{2m}{k_B T}$ then the above sum can be written as an integral of the form

$$\frac{1}{2\pi i}\int_C \frac{\pi}{\sin\pi Z}\,\frac{e^{-C^*HZ}}{\{1+(1-4pqe^{-C^*HZ})^{\frac{1}{2}}\}^3}\,dZ \quad .$$

We now replace the contour C, which encloses the real axis on the positive side excluding the origin, by $C' = \frac{1}{2} + iy$, which is permissible on the positive side of the real axis.

Then

$$\frac{1}{2\pi i}\int_{C'} \frac{\pi}{\sin\pi Z}\,dZ = \frac{1}{2}$$

therefore

$$16q^3 \sum_{n=1}^{\infty} (-1)^{n+1}\,\frac{\mu^n}{\{1+(1-4pq^n)^{\frac{1}{2}}\}^3}$$

$$= 16q^3\{\frac{1}{2} + \frac{1}{2\pi i}\int_{C'} \frac{\pi}{\sin\pi Z}\,dZ\,[\frac{e^{-C^*HZ}}{(1+(1-4pqe^{-C^*HZ})^{\frac{1}{2}})^3} - 1]\}$$

at $p = p_c = \frac{1}{2}$ and for small H

$$2\sum_{n=1}^{\infty} (-1)^{n+1}\,\frac{\mu^n}{\{1+(1-\mu^n)^{\frac{1}{2}}\}^3} = 1 - \frac{1}{\pi i}\int_{C'} \frac{3\pi}{\sin\pi Z}(C^*HZ)^{\frac{1}{2}}dZ \quad (5.24)$$

hence substituting (5.24) into (5.13) we obtain

$$\frac{M}{N} \sim AH^{\frac{1}{2}}$$

where $A = \frac{3m}{\pi i}^{3/2}(\frac{2}{k_B T})^{\frac{1}{2}}\int_{C'} \frac{\pi}{\sin\pi Z}\,Z^{\frac{1}{2}}dZ$.

Hence we obtain a value of $\delta = 2$.

If we had considered the site problem instead this would have introduced a factor p into the argument and at $p = p_c = \frac{1}{2}$ we have

$$\frac{M}{N} \sim \frac{A}{2}\,H^{\frac{1}{2}} \quad .$$

5.2 Calculation of δ for $p = 1$ and $T = T_c$

We may write the partition function Z as

$$\log Z = -\tfrac{1}{2}\log\mu + \log\Lambda(\alpha,z) + f(z)$$

thus

$$k_B T \frac{\partial}{\partial H}\log Z = m + k_B T \frac{\partial}{\partial \alpha}\log\Lambda(\alpha,z).\frac{\partial \alpha}{\partial H} \quad . \tag{5.25}$$

Now the magnetisation $M = m(1 - 2\alpha)$

therefore

$$\frac{\partial M}{\partial H} = -2m\frac{\partial \alpha}{\partial H} = \chi \quad . \tag{5.26}$$

Substituting (5.26) into (5.25) gives

$$M = m - \frac{k_B T}{2m} \frac{\partial}{\partial \alpha} \log\Lambda(\alpha,z).\chi \tag{5.27}$$

$$\frac{2m^2}{k_B T} \cdot \frac{1}{\chi} = \frac{\partial/\partial\alpha \log\Lambda}{1-M/m} \quad .$$

We now use the method of Rushbrooke and Scoins, see [27] page 266, which is exact on the Bethe lattice, to derive $\log \Lambda$. This gives

$$\log\Lambda = -\log(1-\alpha) + \frac{q}{2}\log\{(1-\alpha) + \frac{1}{2}z^2(2\alpha-1+\xi)\} \tag{5.28}$$

where $z = e^{-2J/k_B T}$

$$\xi = [1 + 4\alpha(1-\alpha)f]^{\frac{1}{2}}$$

$$f = 1/z^2 - 1 \quad .$$

From (5.28)

$$\frac{\partial}{\partial\alpha}\log\Lambda = \frac{1}{1-\alpha} + \frac{q}{2}\left\{\frac{\frac{1}{2}z^2(2+\partial\xi/\partial\alpha)-1}{(1-\alpha)+\frac{1}{2}z^2(2\alpha-1+\xi)}\right\} \quad . \tag{5.29}$$

We now replace α by $\frac{1}{2}(1 - \frac{M}{m})$ and after some algebraic manipulation obtain

$$\frac{\partial}{\partial\alpha}\log\Lambda \sim 2(1 - M/m + M^2/m^2)$$

$$+ q\left\{\frac{z^2 - 1 + z(1-z^2)M/m}{1 + z + (1-z^2)M/m - z/2(1-z^2)M^2/m^2}\right\}$$

hence

$$\frac{\partial}{\partial\alpha}\log\Lambda \sim 2(1-M/m+M^2/m^2) + q(1-z)\{-1 + \frac{M}{m} + \frac{1}{2}(z-1)(z+2)\frac{M^2}{m^2}\}$$

now

$$\frac{2m^2}{k_BT} \cdot \frac{1}{\chi} \sim \frac{\partial}{\partial\alpha}\log\Lambda \cdot [1 + M/m - M^2/m^2 + \ldots]$$

hence

$$\frac{2m^2}{k_BT} \cdot \frac{1}{\chi} \sim 2 + q(z-1) + \frac{M^2}{m^2}[\frac{q}{2}(1-z)(z^2+z+2)-2]$$

at $T = T_c$ $z = z_c = \frac{q-2}{q}$ and this becomes

$$\frac{2m^2}{k_BT_c} \cdot \frac{1}{\chi} \sim \frac{M^2}{m^2}(q-1)(q-2) \cdot \frac{2}{q^2} \quad . \tag{5.30}$$

If $H \sim M^\delta$

then $\frac{\partial M}{\partial H} = \chi \sim H^{1/\delta-1}$

therefore

$$\frac{1}{\chi} \sim M^{\delta-1}$$

from (5.30) we see that $\delta = 3$.

The value of δ agrees with the value obtained if we use the conjectured scaling equality

$$\gamma' = \beta(\delta - 1) \quad .$$

On the Bethe lattice $\gamma' = 1$ and $\beta = \frac{1}{2}$ giving a value of $\delta = 3$.

Chapter 6 Proofs of certain results conjectured by J.W. Essam and G.A. Baker Jr.

6.1 Proof that $\sum_{G'} v(G')k(G') = n(G) - B$

Initially we consider the mean number of clusters expansion for a graph G with V vertices

$$K(p;G) = \sum_{j=1}^{V} K'_j p^j \tag{6.10}$$

$$K'_j = \sum_{c_j} k(c_j) \tag{6.11}$$

where c_j is a list of connected subgraphs , see [22], of G with j vertices

$k(c_j)$ is the weak k weight, see [22] and [7], of c_j .

The mean number of clusters may also be written in the form

$$K(p;G) = \sum_{j=1}^{V} s_j p^j \tag{6.12}$$

$$s_j = \sum_{i=1}^{j} a_{ij} \tag{6.13}$$

where a_{ij} are the elements of a matrix $A(G)$

$$a_{ij} = (-1)^{j-i} \sum_{n} \binom{n}{j-i} K_{i,n}(G) \qquad i \leq j$$

$$= 0 \qquad i > j$$

where $K_{i,n}(G)$ is the number of connected section graphs of G, see [22], with i vertices the corresponding clusters of which have perimeter n.

This matrix is effectively derived from the coefficients of binomial expansions of the form $A_n p^i (1-p)^n$, $n = V - i$, such that a_{ij} is the coefficient of p^j derived from the graph with i sites.

If e_ℓ is the number of components of the graph obtained when the ℓ^{th} set of n sites is removed from G then

$$A_n = \sum_\ell e_\ell \quad . \tag{6.14}$$

From equations (6.10), (6.11), (6.12) and (6.13) we see that

$$\sum_{c_j} k(c_j) = \sum_i a_{ij} \quad . \tag{6.15}$$

Therefore

$$\sum_j j \sum_{c_j} k(c_j) = \sum_j j \sum_i a_{ij} \quad . \tag{6.16}$$

The left hand side of equation (6.16) can be re-written in the form

$$\sum_{G'} k(G')v(G')$$

where the sum runs over all connected subgraphs,

$$G' \text{ , of } G$$

and $v(G')$ is the number of vertices in G' .

Therefore

$$\sum_{G'} k(G')v(G') = \sum_i \sum_j j a_{ij} \quad .$$

We now consider the form of the expression from which the a_{ij} are derived, namely $A_n p^i (1-p)^n$ now

$$A_n p^i (1-p)^n = A_n \sum_{r=0}^{n} (-1)^r \binom{n}{r} p^{r+i} \quad . \qquad (6.17)$$

Differentiating (6.17) with respect to p then multiplying throughout by p gives,

$$iA_n p^i (1-p)^n - A_n . n . p^{i+1} (1-p)^{n-1} = A_n \sum_{r=0}^{n} (-1)^r (r+i) \binom{n}{r} p^{r+i}$$

for $n \geq 2$ and $p = 1$ the right hand side of the above equation is zero.

Therefore

$$A_n \sum_{r=0}^{n} (-1)^r (r+i) \binom{n}{r} = 0 \qquad n \geq 2 \quad .$$

Hence

$$\sum_j j a_{ij} = 0 \qquad \text{for graphs with perimeter greater than one.}$$

Therefore the only contribution to the sum $\sum_i \sum_j j a_{ij}$ is from graphs with perimeter one and perimeter zero.

$$\sum_{G'} k(G')v(G') = \sum_j j a_{v-1,j} + \sum_j j a_{v,j} \quad .$$

The contribution for graphs with perimeter one is derived from

$$A_1 p^{V-1}(1-p) \quad .$$

Therefore

$$\sum_j j a_{V-1,j} = A_1(V-1) - A_1 V$$

$$= -A_1 \quad .$$

The only subgraph with zero perimeter is the graphs itself, hence,

$$\sum_j j a_{V,j} = n(G).V$$

where $n(G)$ are the number of components in the graph G .

From the previous definition of A_n given in (6.14)

$$A_1 = \{n(G)V - n(G)a + x\} - K \qquad (6.18)$$

where

a is the number of articulation points in G

K is the number of isolated vertices in the graph G .

If d_i is the number of blocks attached to the i^{th} articulation point then

$$x = \sum_i \{d_i + n(G) - 1\}$$

$$= \sum_i d_i + an(G) - a \quad .$$

Let $Y = \sum_i d_i$.

Then we consider the relation

$$Y_m = b_m + a_m - n_m \tag{6.19}$$

where b_m is the number of blocks in the graph

a_m is the number of articulation points

n_m is the number of components.

m is used here as an ordering parameter; e.g. b_{m+1} is simply the number of blocks contained in the graph, which is derived by adding one block to the graph with b_m blocks.

This is necessary since we seek to use an inductive proof to show the truth of (6.19). We assume the truth of (6.19) and show that the relation is true for Y_{m+1}. To do this three cases must be considered.

(i) An extra block is attached to an already existing articulation point.

(ii) An extra block is attached to any site other than an articulation point.

(iii) The extra block forms a new component.

For (i)

$$\begin{aligned} Y_{m+1} &= Y_m + 1 \\ &= b_m + a_m + 1 - n_m \quad . \end{aligned} \tag{6.20}$$

Now

$$b_m = b_{m+1} - 1$$

$$a_m = a_{m+1}$$

$$n_m = n_{m+1} \quad .$$

Therefore substituting in (6.20) gives

$$Y_{m+1} = b_{m+1} + a_{m+1} - n_{m+1} \quad .$$

For (ii)

$$Y_{m+1} = Y_m + 2$$

and

$$b_m = b_{m+1} - 1$$

$$a_m = a_{m+1} - 1$$

$$n_m = n_{m+1} \quad .$$

Therefore for this case also

$$Y_{m+1} = b_{m+1} + a_{m+1} - n_{m+1} \quad .$$

For (iii)

$$Y_{m+1} = Y_m$$

and

$$b_m = b_{m+1} - 1$$

$$a_m = a_{m+1}$$

$$n_m = n_{m+1} - 1 \quad .$$

Therefore again we see that

$$Y_{m+1} = b_{m+1} + a_{m+1} - n_{m+1} \quad .$$

Hence if the relationship is true for Y_m we have shown that it is true for Y_{m+1} .

It if necessary now to show the truth of (6.19) for Y_m and to do this we consider a graph with no articulation points and which has only one component; i.e. a star graph.

From the definition $Y_m = 0$

now for this graph $b_m = 1$

$$a_m = 0$$

$$n_m = 1$$

hence

$$Y_m = b_m + a_m - n_m \quad .$$

It follows that since the statement is true for this graph it is true for all graphs.

Hence

$$x = b + a - n(G) + a.n(G) - a$$

$$= b - n(G)[1 - a]$$

and

$$A_1 = n(G)V + b - n(G) - K \quad .$$

Since

$$\sum_{G'} k(G')v(G') = n(G)V - A_1$$

$$= -b + n(G) + K \qquad V \geq 2 \quad .$$

Then

$$\sum_{G'} k(G')v(G') = n(G) - B \qquad V \geq 2 \tag{6.21}$$

where B is the number of blocks in the graph excluding single vertices.

If G is the single vertex then it can be seen than (6.21) is satisfied for this graph and the restriction $V \geq 2$ can be removed.

Since

$$\sum_{G'} k(G') = n(G)$$

from (6.21)

$$\sum_{G'} k(G')[v(G') - 1] = -B$$

for a graph G' with only one component $v(G') - 1$ is the cocycle rank, see [22], hence

$$\sum_{G'} k(G')r(G') = -B \quad . \tag{6.22}$$

6.2 Proof that $\sum_{G'} k(G')v^2(G') = \sum_{b'} \sum_{j=1}^{V(b')} f_j - V - 2(b - n(G))$

From similar arguments to those given in the previous section 6.1 we have

$$\sum_{G'} v^2(G')k(G') = \sum_i \sum_j j^2 a_{ij}$$

and

$$\sum_i \sum_j j^2 a_{ij} = 0 \quad \text{for all graphs with perimeter greater than two.}$$

The contribution for graphs with perimeter two is derived from

$$A_2 p^{V-2}(1-p)^2 \quad .$$

Therefore

$$\sum_j j^2 a_{V-2,j} = A_2\{(V-2)^2 - 2(V-1)^2 + V^2\}$$

$$= 2A_2 \quad .$$

The contribution for graphs with perimeter one is derived from

$$A_1 p^{V-1}(1-p) \quad .$$

Therefore

$$\sum_j j^2 a_{V-1,j} = A_1\{(V-1)^2 - V^2\}$$

$$= A_1(1-2V) \quad .$$

The contribution for graphs with zero perimeter is $n(G)V^2$.

Hence

$$\sum_{G'} v^2(G')k(G') = 2A_2 + A_1(1-2V) + n(G)V^2 \quad .$$

For 1- irreducible graphs, see [6]

$A_1 = V$, $n(G) = 1$ and $b = 1$.

Then

$$\sum_{G'} v^2(G')k(G') = 2A_2 + V(1-V) \quad . \qquad (6.23)$$

Let a' be the number of articulation pairs

c_i' be the number of components the graph splits into when the i^{th} articulation pair is removed

$$x' = \sum_i c_i' \quad .$$

Now

$$A_2 = \{\frac{V(V-1)}{2} + x' - a'\} \quad .$$

Substituting A_2 in (6.23) gives

$$\sum_{G'} v^2(G')k(G') = 2(x'-a') \quad . \tag{6.24}$$

When the j^{th} vertex is removed, let the section graph containing the remaining vertices of G contain e_j articulation points and f_j blocks.

Then from (6.19)

$$x_j = e_j + f_j - 1$$

and

$$a' = \tfrac{1}{2} \sum_{j=1}^{V} e_j$$

$$x' = \tfrac{1}{2} \sum_{j=1}^{V} x_j \quad .$$

Therefore

$$2x' - 2a' = \sum_{j=1}^{V} f_j - V \qquad V \geq 3 \tag{6.25}$$

$$\sum_{G'} v^2(G')k(G') = \sum_{j=1}^{V} f_j - V \quad . \tag{6.26}$$

(6.26) is true for 1- irreducible graphs but a graph which is not 1- irreducible can be split into its separate blocks and the sum performed over each block in turn. This is possible provided account is taken of the extra number of sites added and of each bond block.

Now $\sum_{G'} v^2(G')k(G') = -2$ if G is the bond and in splitting the graph into its separate blocks $b - n(G)$ sites are added.

If there are m bond blocks in the graph G then

$$\sum_{G'} v^2(G')k(G') = \sum_{b'} \{ \sum_{j=1}^{v(b')} f_j - v(b') \} - 2m - b + n(G)$$

where b' is the number of blocks containing more than two vertices, i.e. $b' = b - m$

$v(b')$ is the number of sites contained in b' .

Now

$$\sum_{b'} v(b') = V + b - n(G) - 2m \quad .$$

Therefore

$$\sum_{G'} v^2(G')k(G') = \sum_{b'} \sum_{j=1}^{V(b')} f_j - V - 2[b-n(G)]$$

$V \geq 2$ for each component .

In all the previous expression we have used the weak k weight $k(G')$ and summed over all the connected subgraphs G' of G . However (6.11) may also be written as

$$K'_j = \sum_{c_j} K(c_j)$$

where now c_j is a list of connected section graphs of G with j vertices

$K(c_j)$ is the strong K weight.

We see that the results derived are then equally true for the strong K weight, e.g.

$$\sum_{G^*} v(G^*)K(G^*) = n(G) - B$$

where the sum G^* is now taken over all connected section graphs of G. Similarly for the other results derived.

Appendix I

Distribution of cluster size for various two and three dimensional lattices.

t = perimeter , s = size .

The matrix a(L) , as far as is known, for each lattice is also included.

Hexagonal Matching Lattice - Site Problem

The count is doubled to avoid fractions.

t^s	1	2	3	4	5	6	7	8
12	2							
13								
14		3						
15		0						
16		0	6					
17		6	0					
18		3	0	14		1		
19			26	0	6	0		
20			6	9	30	0	6	
21			2	78	0	36	0	
22			30	15	66	63	0	
23			12	36	216	0	174	
24			6	171	42	393	124	
25			6	66	336	532	222	
26				69	624	309	1554	
27				124	312	1738	1314	
28				84	678	2088	2490	
29				30	930	1914	7380	
30				14	702	4356	7094	
31					648	4726	12930	
32					618	5049	20280	
33					480	5826	23828	
34					252	6343	33576	
35					84	6018	38130	
36					30	4617	46432	
37						3884	50802	
38						2928	46380	
39						1650	49512	
40						738	44604	

Hexagonal Matching Lattice (Cont.)

t^s	1	2	3	4	5	6	7	8
41						228	33696	
42						63	25898	
43							19128	
44							10974	
45							5384	
46							2172	
47							576	
48							124	

Simple Quadratic Matching Lattice - Site Problem

t^s	1	2	3	4	5	6	7	8
8	1							
9								
10		2						
11		0						
12		2	6	1				
13			0	0				
14			8	18	8	2		
15			4	8	4	0		
16			2	12	55	40	22	
17				1	60	58	20	
18				24	116	186	170	
19				8	100	300	404	
20				2	145	570	864	
21					84	510	1384	
22					52	742	2692	
23					12	620	3012	
24					2	458	3744	
25						236	3704	
26						92	3428	
27						16	2168	
28						2	1292	
29							0	
30							0	
31							20	
32							2	

Triangular Lattice - Site Problem

t^s	1	2	3	4	5	6	7	8	9
6	1								
7									
8		3							
9			2						
10			9	3					
11				12	6				
12				29	21	14	1		
13					66	43	30	6	
14					93	153	111	69	27
15						298	366	291	166
16						306	840	957	803
17							1290	2349	2592
18							1014	4299	6734
19								5310	13634
20								3408	20469
21									21372
22									11562

Simple Quadratic Lattice - Bond Problem

Counts per site

t^s	1	2	3	4	5	6	7	8	9	10
6	2									
7										
8		6		1						
9			4	0						
10			18	0	8		2			
11				32	0	14	0			
12				55	30	40	0	22		6
13					160	0	156	0	60	0
14					174	332	168	228	134	62
15						672	336	958	164	728
16						570	2030	869	2776	656
17							2712	4064	4724	5308
18							1908	9972	8770	18816
19								10880	27392	27540
20								6473	46004	74576
21									43220	148728
22									22202	207444
23										169784
24										76886

Simple Quadratic Lattice - Site Problem

t^s	1	2	3	4	5	6	7	8	9	10
4	1									
5										
6		2								
7			4							
8			2	9	1					
9				8	20	4				
10				2	28	54	22	4		
11					12	80	136	80	28	4
12					2	60	252	388	291	154
13						16	228	776	1152	986
14						2	100	818	2444	3676
15							20	480	280	7612
16							2	152	2089	9750
17								24	856	8192
18								2	216	4330
19									28	1416
20									2	292
21										32
22										2

Simple Quadratic Lattice - Site Problem (Cont.)

t^s	11	12	13
12	52	9	1
13	644	325	112
14	3530	2644	1660
15	1177	12502	10480
16	24472	38694	44574
17	33336	79730	129020
18	31202	114342	264482
19	19532	115502	391432
20	8130	83183	423786
21	2180	41136	337144
22	380	14064	193820
23	36	3208	79240
24	2	480	22993
25		40	4508
26		2	592
27			44
28			2

Simple Cubic Lattice with first, second and third neighbours - Site Problem

t^s	1	2	3	4	5	6	7
26	1						
27							
28							
29							
30							
31							
32							
33							
34		3					
35		0					
36		0					
37		0					
38		0					
39		0					
40		6					
41		0					
42		0	15				
43		0	0				
44		4	0	3			
45			0	0			
46			0	0			
47			0	0			
48			48	0			
49			0	0			
50			8	83			
51			12	0			
52			24	30	48		
53			0	24	0		
54			30	0	24	18	

Simple Cubic Lattice with first, second and third neighbours (cont.)

t^s	1	2	3	4	5	6	7
55			0	0	12	0	
56			48	326	8	16	
57			12	0	0	0	
58			24	120	510	0	
59			0	147	0	0	
60			0	264	360	480	
61			12	120	432	0	
62			4	384	288	480	
63				0	240	510	
64				480	2172	390	
65				360	132	336	
66				348	1368	3471	
67				168	1782	264	
68				380	2348	3612	
69				276	2004	4956	
70				492	4833	4536	
71				138	1296	5376	
72				276	4896	18174	
73				144	4560	5328	
74				216	4940	15472	
75				96	4104	20593	
76				48	7362	24300	
77				8	4836	26124	
78				36	9132	52116	
79				24	5310	28620	
80				4	5812	59744	
81					5772	63080	
82					7602	69174	
83					5396	66568	
84					6456	106446	
85					3192	83416	

t^s	1	2	3	4	5	6	7
86					5166	131528	
87					3216	108783	
88					3060	122538	
89					1548	124172	
90					1260	157440	
91					1296	125760	
92					698	158528	
93					348	123120	
94					144	146406	
95					108	130236	
96					108	130554	
97					36	104184	
98					4	105460	
99						86094	
100						88908	
101						58832	
102						53082	
103						37308	
104						33348	
105						23724	
106						14532	
107						8436	
108						7716	
109						4896	
110						2276	
111						1032	
112						588	
113						432	
114						216	
115						48	
116						4	

Face Centred Cubic Lattice - Site Problem

t^s	1	2	3	4	5	6	7	8
12	1							
13								
14								
15								
16								
17								
18		6						
19								
20								
21								
22			8					
23			12					
24			30	2				
25				0				
26				27				
27				48				
28				96	24			
29				144	6			
30				158	132	6		
31					264	24		
32					423	145		
33					780	168	36	
34					1194	914	80	
35					1212	1308	288	
36					846	2688	1220	
37						5000	1968	
38						7140	5382	
39						10272	10308	
40						11340	18918	

Face Centred Cubic Lattice - Site Problem (cont.)

t^s	1	2	3	4	5	6	7	8
41						9168	31128	
42						4662	53616	
43							75528	
44							93852	
45							110680	
46							98496	
47							65700	
48							26182	

Face Centred Cubic Lattice - Bond Problem

t^s	1	2	3	4	5	6	7
22	6						
23							
24							
25							
26							
27							
28							
29							
30			8				
31		24	0				
32		42	0				
33			0				
34			0				
35			0				
36			0			2	
37			0		12	0	
38			0	30	24	0	
39			32	120	0	0	
40			192	123	0	0	
41			372	0	0	0	
42			326	0	0	0	
43				0	0	0	
44				0	0	0	
45				0	0	0	240
46				0	0	816	96
47				0	1464	648	0
48				1230	1728	504	0
49				1896	2616	0	0
50				4176	1512	0	0
51				4584	0	0	0
52				2739	0	0	0

t^s	1	2	3	4	5	6	7
53					0	0	744
54					0	740	9048
55					384	10488	17736
56					6168	25080	23088
57					17256	42600	15792
58					35880	43536	7770
59					47784	41298	0
60					65550	17648	0
61					53640	0	0
62					24234	0	32568
63						13456	74832
64						33960	326400
65						167472	580704
66						339088	778632
67						534336	949176
68						798972	809040
69						881496	591156
70						934992	200904
71						612000	202440
72						222566	405120
73							1743264
74							3379560
75							6531792
76							9395856
77							12568800
78							14886168
79							14582112
80							12582594
81							6902880
82							2102208

Body Centred Cubic Lattice - Site Problem

t^s	1	2	3	4	5	6	7	8
8	1							
9								
10								
11								
12								
13								
14		4						
15								
16								
17			12					
18			0					
19			12					
20			4	42				
21				0	6			
22				78	0			
23				32	152			
24				36	30	51		
25				24	408	24	12	
26				4	182	632	16	
27					384	204	324	
28					336	2088	144	
29					144	1352	3096	
30					108	2748	2058	
31					36	2568	10416	
32					4	2112	8774	
33						2016	18408	
34						1044	18438	
35						480	20884	
36						216	20820	
37						48	15024	

t^s	1	2	3	4	5	6	7	8
38						4	11184	
39							6756	
40							2820	
41							1148	
42							360	
43							60	
44							4	

Hexagonal Matching Lattice - Site Problem. The count is doubled to avoid fractions.

2	-24	132	-440	990	-1584	1848	-1584	990
0	12	-198	1548	-7620	26463	-68838	138957	-222456
0	0	88	-1832	18348	-117650	542202	-1911090	5351898
0	0	0	710	-17766	215772	-1693928	9657576	-42590442
0	0	0	0	6054	-176496	2512098	-23255334	157380300
0	0	0	0	0	53500	-1778174	28972491	-308357768
0	0	0	0	0	0	484784	-18075960	331406178
0	0	0	0	0	0	0	4475010	-184870815
0	0	0	0	0	0	0	0	41902042

Simple Quadratic Matching Lattice - Site Problem.

1	-8	28	-56	70	-56	28	-8	1
0	4	-44	222	-680	1410	-2088	2268	-1824
0	0	20	-276	1784	-7172	20078	-41516	65604
0	0	0	110	-1813	14180	-69988	244511	-642768
0	0	0	0	628	-12192	111546	-650288	2712085
0	0	0	0	0	3832	-83168	869770	-5836188
0	0	0	0	0	0	23592	-572676	6731068
0	0	0	0	0	0		147941	-3968963
0	0	0	0	0	0			940982

Body Centred Cubic Lattice - Site Problem.

1	-8	28	-56	70	-56	28	-8	1
0	4	-56	364	-1456	4004	-8008	12012	-13728
0	0	28	-512	4444	-24348	94452	-275808	629136
0	0	0	216	-4860	52530	-363136	1803356	-6850372
0	0	0	0	1790	-47710	615506	-5119744	30858014
0	0	0	0	0	15587	-479596	7180100	-69691516
0	0	0	0	0	0	140746	-4905608	83513644
0	0	0	0	0	0	0	1305920	0
0	0	0	0	0	0	0	0	0

Simple Cubic Lattice with 1st, 2nd and 3rd neighbours - Site Problem.

1	-26	325	-2600	14950	-65780	230230
0	13	-518	10147	-130208	1230472	-9126848
0	0	237	-12558	329181	-5689012	72891080
0	0	0	4995	-328293	10709544	-231132233
0	0	0	0	114219	-8937798	347847309
0	0	0	0	0	2753781	-249622454
0	0	0	0	0	0	68911048

Face Centred Cubic Lattice - Site Problem

1	-12	66	-220	495	-792	924	-792	495
0	6	-108	918	-4896	18360	-51408	111384	-190944
0	0	50	-1172	13164	-94292	483560	-1889580	5846148
0	0	0	475	-13650	189657	-1696800	10983036	-54787656
0	0	0	0	4881	-165738	2737290	-29294784	228353700
0	0	0	0	0	52835	-2066952	39496762	-491239292
0	0	0	0	0	0	593382	-26255336	569238018
0	0	0	0	0	0	0	6849415	
0	0	0	0	0	0	0	0	

Face Centred Cubic Lattice - Bond Problem

6	-132	1386	-9240	43890	-158004	447678	-1023264	1918620
0	66	-2088	31992	-316200	2265480	-12535656	55730808	-204475752
0	0	930	-38112	762678	-9929888	94559772	-701995632	4228905668
0	0	0	14898	-747696	18415200	-296614284	3513166011	-32621254308
0	0	0	0	258252	-15314856	447174042	-8568393912	121161248880
0	0	0	0	0	4721698	-322728966	10886821638	-241595656034
0	0	0	0	0	0	89700720	-6938268168	265338364194
0	0	0	0	0	0	0	1753975176	-151385289636
0	0	0	0	0	0	0		35076310294

Appendix II

Calculation of the Möbius function for a given lattice.

We define the lattice $L(G)$ of any connected graph $G = (V,E)$ to be the set of subsets of E ordered by containment and having the following properties:

(a) $\overline{E'} = E$ where $\overline{E'}$ is the bond closure of E'

(b) $G' = (V,E')$ is connected and has exactly one multiply connected block.

We show that:

For all graphs $G' \in L(G)$

$$\mu(E',E'') = \begin{cases} (-1)^{|E''-E'|} & \text{if } E' \subseteq E'' \text{ ; } \overline{E'} = E'' \\ & \text{and all graphs obtained from} \\ & G' \text{ are elements of } L(G) \\ 0 & \text{otherwise .} \end{cases}$$

All graphs obtained from G' are those graphs obtained by adding to G' all combinations of edges from the edge set $E'' - E'$.

The set of all graphs with more than one multiply connected block will be referred to as ξ

(i) We first show that for all graphs G' , where all graphs obtained from G' are allowed, has Möbius function:

$$\mu(E',E'') = (-1)^{|E''-E'|}$$

now

$$\sum_{E' \subseteq E''' \subseteq E''} \mu(E''',E'') = 0$$

hence

$$\mu(E',E'') = - \sum_{E' \subset E''' \subseteq E''} \mu(E''',E'') \quad . \qquad (1)$$

The proof is an inductive one and we assume that the required result is true for all graphs $G''' = (V,E''')$.

Let $|E'' - E'| = n$.

From (1)

$$\mu(E',E'') = -\{n(-1)^{n-1} + {}^{n}C_{2}(-1)^{n-2} + \ldots + {}^{n}C_{r}(-1)^{n-r} + \ldots + 1\} \quad . \qquad (2)$$

Consider the expansion of $(1+x)^n$

$$(1+x)^n = 1 + nx + \ldots + {}^{n}C_{r}x^{r} + \ldots + x^{n}$$

for $x = -1$.

$$0 = 1 + n(-1) + \ldots + {}^{n}C_{r}(-1)^{r} + \ldots + (-1)^{n}$$

hence the left hand side of (2) is $(-1)^{n+2} = (-1)^{n}$. Therefore $\mu(E',E'') = (-1)^{|E''-E'|}$ if the result is true for all G''' .

Now the Möbius function of the first graph $G'' = (V,E'')$ is $1 = (-1)^{0}$. Since the assumed result holds for the first graph by induction it holds for all the G''' and the required result follows.

(ii) To complete the proof we consider a graph $G' = (V,E')$ such that not all the graphs obtained from G' are elements of $L(G)$.

We assume that $\mu(E"',E") = 0$, $E' \subset E"' \subset E"$. If a member of ξ can be obtained from $G"'$.

We have shown that $\mu(E"',E") = (-1)^{|E"-E"'|}$ otherwise .

Let $|E"-E'| = n$.

Let there be m ways of adding one edge to G' such that a member of ξ is obtained then

$$\mu(E',E") = -\{[n - m - \sum_{il} 1](-1)^{n-1}$$

$$+[{}^{n}C_{2} - {}^{m}C_{2} - \sum_{il} P_{il} - \sum_{i2} 1](-1)^{n-2} + \ldots$$

$$+[{}^{n}C_{r} - B_{r} - \sum_{ir} 1](-1)^{n-r} + \ldots + 1\}$$

$$B_{r} = \sum_{il}^{P_{il}} C_{r-1} + \sum_{i2}^{P_{i2}} C_{r-2} + \ldots + \sum_{i(r-1)}^{P_{i(r-1)}} .$$

B_r contains all those graphs which can be obtained from G' by adding r edges from the edge set $E"-E'$, and which are not elements of $L(G)$;

$\sum_{ir} 1$ is the sum over all the graphs $G"'$ which have $\mu(E"',E") = 0$ and $|E"' - E"| = r$;

$\sum_{ik}^{P_{ik}} C_{r-k}$ is such that the sum is taken over the set of graphs $G"'$ where $\mu(E"',E") = 0$ and $|E"',E'| = k$;

and P_{ik} is the number of ways in which one edge can be added to the i^{th} graph of the set G''', defined above, to give a member of the set ξ.

All expressions of the form ${}^{n}C_{r}$ are defined to be 0 if $r > n$.

Consider the following sum

$$\sum_{ir} 1 - \sum_{ir} P_{ir} + \sum_{ir} {}^{P_{ir}}C_2 + \ldots + (-1)^k \sum_{ir} {}^{P_{ir}}C_k + \ldots + \sum_{ir} (-1)^{P_{ir}}.1$$

$$= \sum_{ir} [1 - P_{ir} + {}^{P_{ir}}C_2 + \ldots + (-1)^{P_{ir}}]$$

$$= 0 \quad .$$

Since this is just the alternating sum of the binomial coefficients. Hence we see immediately that

$$\mu(E',E'') = [n-m](-1)^{n-1} + \ldots + [{}^{n}C_r - {}^{m}C_r](-1)^{n-r}$$

$$+ \ldots + [{}^{n}C_m - 1](-1)^{n-m} + \ldots + 1$$

$$= [(-1)^n - (-1)^n]$$

$$= 0 \quad .$$

Therefore $\mu(E',E'')$ is zero if the initial assumption is correct.

To show that the assumption is correct it is only necessary to consider the set of graphs G''', $E' \subset E''' \subset E''$, such that there is only one way to add an edge to G''' to get a graph $\in \xi$,

and that adding more than one edge leads to an element of $L(G)$. The required result then follows by induction.

Since only one edge can be added to $G"'$ to give a member of ξ , there can be no graph G^* , $E"' \subset E^* \subset E"$ to which bonds can be added to give a member of ξ .

Let $|E" - E"'| = S$

then

$$\mu(E"',E") = \{(S-1)(-1)^{S-1} + \ldots + {}^{S}C_{r}(-1)^{S-r} + \ldots + 1\}$$

$$= 0 \quad .$$

It follows immediately that $\mu(E',E") = 0$ if not all the graphs obtained from G' are elements of $L(G)$, and this completes the proof.

The series of Appendix III has recently been computed by C.J. Elliott, J.L. Martin and M.F. Sykes by the perimeter method.

They agree with our results as far as p^{12} but find $1404p^{13} + 2904p^{14} + 3522p^{15} + 6876p^{16} + 7548p^{17}$.

We have found certain errors in the second moment weights which have now been corrected and we have confirmed their coefficient of p^{13}. However we now find $2964p^{14}$ so that we still appear to have further errors in this and the subsequent term. Since their method is self checking their series is probably correct unless they have at least two compensating errors.

Appendix III

a) Mean size series for the hexagonal lattice site problem

$$S(p) = 1 + 3p + 6p^2 + 12p^3 + 24p^4 + 33p^5 + 60p^6 + 99p^7$$
$$+ 156p^8 + 276p^9 + 438p^{10} + 597p^{11} + 1134p^{12}$$
$$+ 1524p^{13} + 3228p^{14} + 4353p^{15} \quad .$$

The above series was derived from the following list of graphs. Where a 'spike' is attached to a graph, this indicates that a chain of any length may be attached to the graph at any point, unless otherwise shown.

The graphs are listed together with their strong second moment weights.

2

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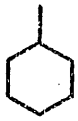

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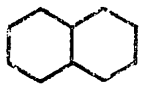

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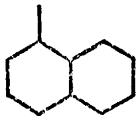

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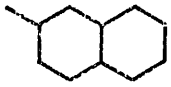

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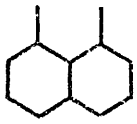

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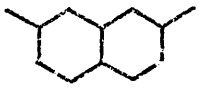

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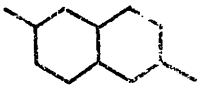

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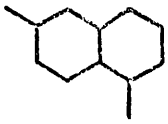

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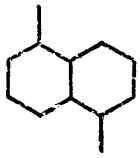

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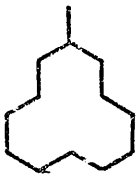

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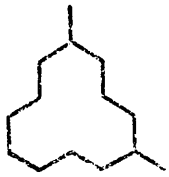

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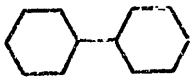

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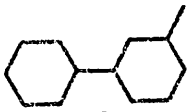

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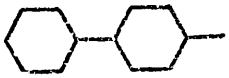

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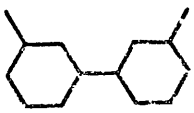

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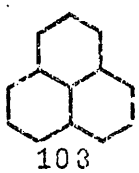

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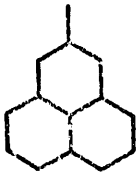

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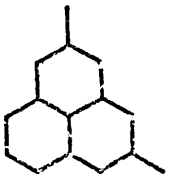

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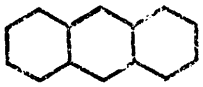

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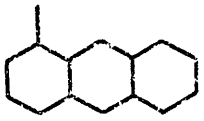

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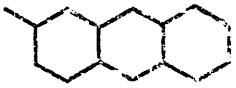

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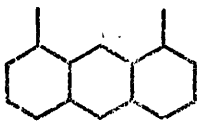

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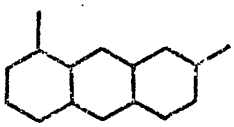

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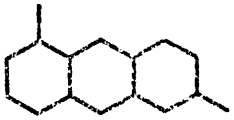

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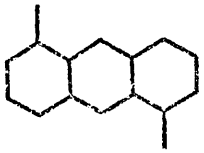

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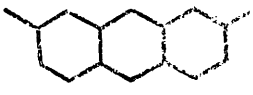

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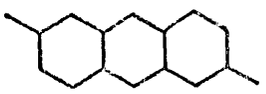

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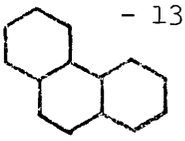

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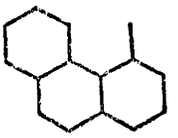

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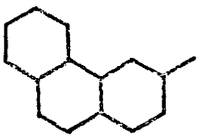

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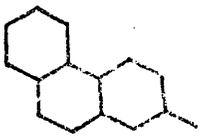

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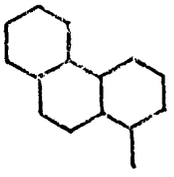

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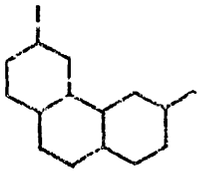

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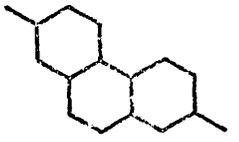

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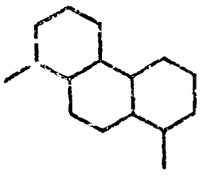

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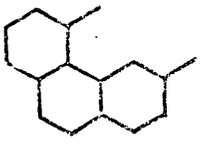

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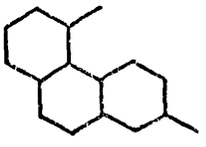

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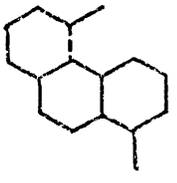

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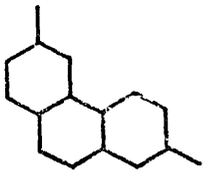

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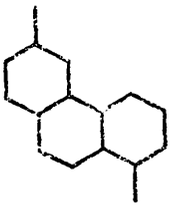

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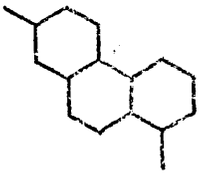

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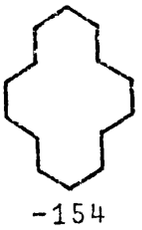

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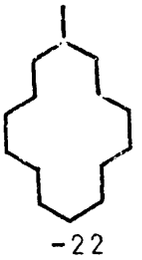

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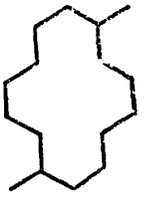


-2

b) The following series are those derived for the site problem using definitions (ii) and (iii) in section 3.1

$$S(p) = \sum_{n=1}^{\infty} a_n p^n$$

$a_n(2)$ will indicate the coefficients derived using (ii)

$a_n(3)$ will indicate the coefficients derived using (iii) .

Simple Quadratic Lattice

n	$a_n(2)$	$a_n(3)$
1	4	2
2	12	12
3	28	32
4	60	68
5	124	144
6	260	300
7	428	520

Triangular Lattice

n	$a_n(2)$	$a_n(3)$
1	6	3
2	24	30
3	66	90
4	174	240
5	432	612
6	1062	1512
7	2490	3618

Hexagonal Matching Lattice

n	$a_n(2)$	$a_n(3)$
1	24	12
2	198	264
3	972	1542
4	4422	7020
5	18936	31038
6	77886	130560

Simple Quadratic Matching Lattice

n	$a_n(2)$	$a_n(3)$
1	8	4
2	44	56
3	156	226
4	516	752
5	1616	2428
6	4896	7472

c) High density mean number series on the honeycomb lattice

$$K(q) = q^3 + \tfrac{1}{2}q^4 + 0q^5 + \tfrac{3}{2}q^6 - 4q^7 + 33q^8 - 73q^9 \quad .$$

The cluster size is distributed as follows:

$q^3(p)$

$q^4(3/2p^2)$

$q^5(3p^3)$

$q^6(7p^4 + 3p^5 + \tfrac{1}{2}p^6)$

$$q^7(15p^5 + 15p^6 + 3p^7)$$

$$q^8(31\tfrac{1}{2}p^6 + 60p^7 + 37\tfrac{1}{2}p^8 + 12p^9 + 1\tfrac{1}{2}p^{10})$$

$$q^9(62p^7 + 177p^8 + 190p^9 + 111p^{10} + 39p^{11} + 9p^{12} + p^{13}) \quad .$$

Appendix IV

a) The following list of graphs are those used to derive the seven bond perimeter polynomial on the face centred cubic lattice. All the graphs required, except the seven bond trees are included, these being enumerated by a different method.

The first figure in the top line of figures for each graph is the count per site of the graph, the second being the count of the graph with one bond added etc.

The second row of figures is the yield factor for the graph, e.g. for the triangle $Y(x) = 1 + 3x$.

Any graph marked with a star indicates that when bonds are added they may be placed at the articulation point also, e.g. when one bond is added to  this will include  .

b) The flow chart and program is that used to count all trees of eight sites.

pq^{22}

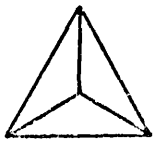
6 42 326 2739 24234 222566

1

p^3q^{30}

8 120 1464 17008 192936

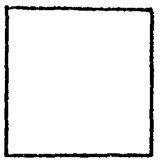
1 3



p^6q^{36}

2 24 276 3120

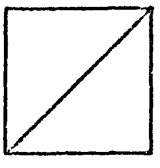
1 6 15 16



p^4q^{40}

3 48 612 7344

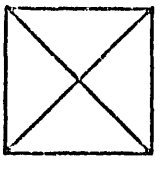
1 4



p^5q^{38}

24 408 5376 65784

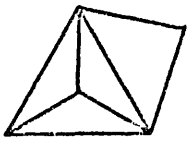
1 5 8



p^8q^{44}

6 120 1716

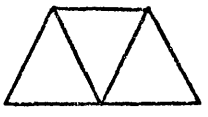
1 8 28 52 45



p^8q^{44}

24 360 4560

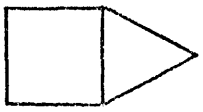
1 8 27 48 40



p^7q^{46}

72 1320 18288

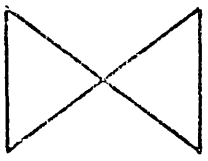
1 7 19 21



p^6q^{48}

24 408 5472

1 6 11



* p^6q^{48}

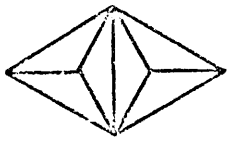
72 1932 35988

1 6 9

$p^{12}q^{48}$

1 24

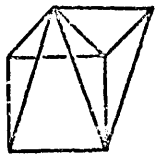
1 12 66 220 489 744 740 384



$p^{11}q^{50}$

6 84

1 11 55 161 296 336 192



$p^{11}q^{50}$

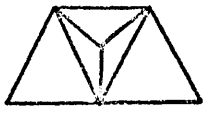
24 408

1 11 55 162 303 353 209

$p^{10}q^{52}$

24 432

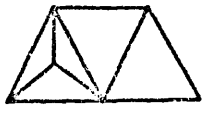
1 10 43 104 146 100



$p^{10}q^{52}$

72 1296

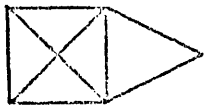
1 10 43 103 144 99



$p^{10}q^{52}$

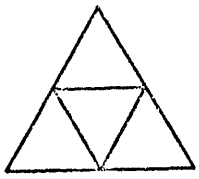
48 768

1 10 44 108 153 104



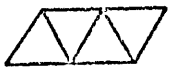
$p^{10}q^{52}$ 24 504

1 10 44 110 161 114



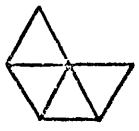
$p^{9}q^{54}$ 32 624

1 9 33 63 54



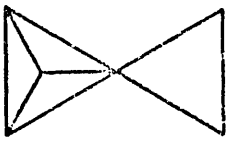
$p^{9}q^{54}$ 120 2400

1 9 34 65 55



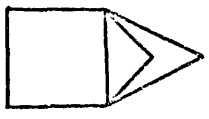
$p^{9}q^{54}$ 120 2448

1 9 34 65 55



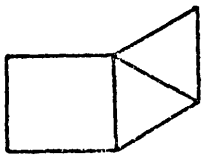
* $p^{9}q^{54}$ 24 696

1 9 33 61 48



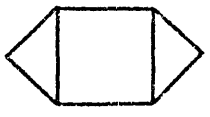
$p^{8}q^{56}$ 12 240

1 8 23 28



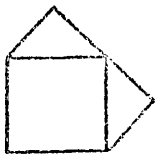
$p^{8}q^{56}$ 96 1872

1 8 24 29



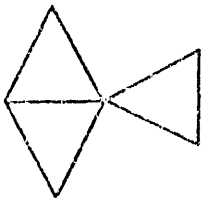
$p^{8}q^{56}$ 24 432

1 8 25 30



p^8q^{56} 48 840

1 8 25 30



p^8q^{56} 144 4464

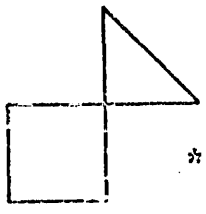
1 8 23 24

p^8q^{56} 288 8304

1 8 23 24

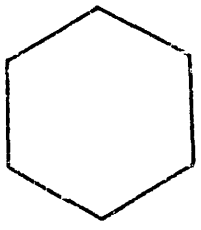
p^7q^{58} 6 108

1 7 15



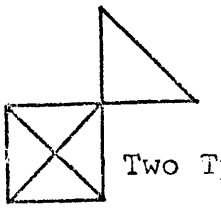
p^7q^{58} 48 1392

* 1 7 12



p^6q^{60} 28 552

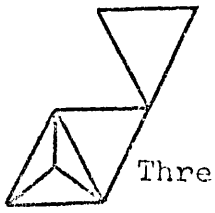
1 6



$p^{11}q^{62}$ 120

1 11 52 136 201 135

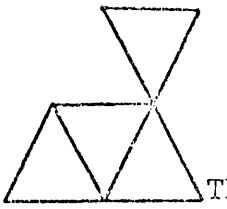
Two Types



$p^{11}q^{62}$ 336

1 11 51 129 184 120

Three Types

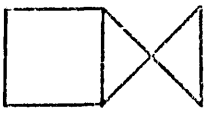


1296

$p^{10}q^{64}$

1 10 40 78 63

Three Types

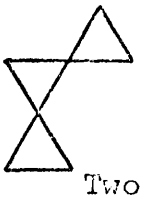


384

$p^{9}q^{66}$

1 9 29 33

Three Types

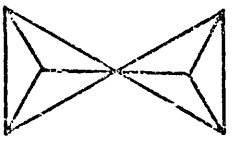


768

$p^{9}q^{66}$

1 9 27 27

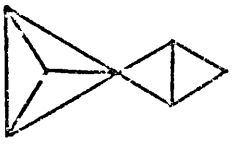
Two Types



4

$p^{12}q^{60}$

1 12 66 212 417 480 256

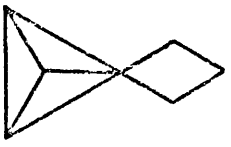


48

$p^{11}q^{62}$

1 11 53 139 200 128

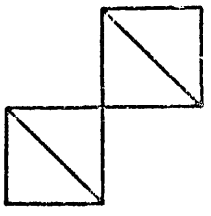
Two Types



0

$p^{10}q^{64}$

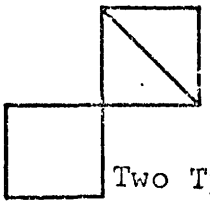
1 10 39 76 64



636

$p^{10}q^{64}$

1 10 41 80 64

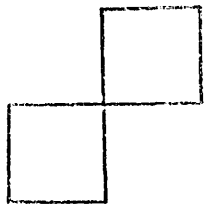


144

$p^{9}q^{66}$

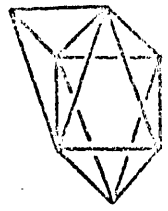
1 9 28 32

Two Types



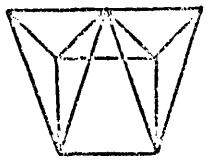
$p^{8}q^{68}$ 12

1 8 16



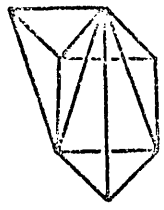
$p^{15}q^{54}$ 8

1 15 105 454 1350 2901 4583 5250 4071 1682



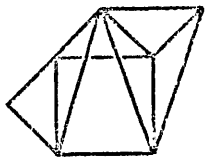
$p^{14}q^{56}$ 12

1 14 91 362 975 1846 2443 2122 960



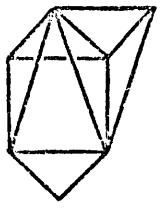
$p^{14}q^{56}$ 24

1 14 91 361 966 1812 2377 2057 935



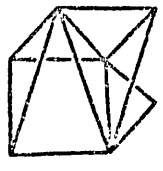
$p^{13}q^{58}$ 24

1 13 77 274 643 1015 1025 528



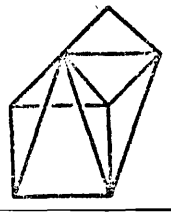
$p^{13}q^{58}$ 48

1 13 77 273 637 1001 1011 523



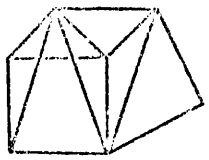
$p^{13}q^{58}$ 24

1 13 77 272 629 977 977 506



$p^{13}q^{58}$ 48

1 13 77 273 635 991 993 513

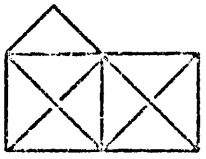


$p^{13}q^{58}$ 96

1 13 77 273 636 996 1000 516

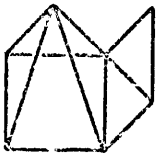
$p^{13}q^{58}$ 24

1 13 77 273 634 982 964 480



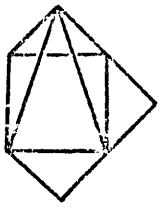
$p^{13}q^{58}$ 48

1 13 77 272 627 963 943 472



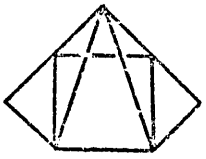
$p^{12}q^{60}$ 96

1 12 65 206 411 500 297



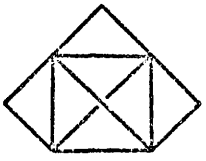
$p^{12}q^{60}$ 24

1 12 64 199 392 477 287



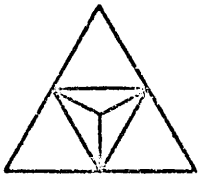
$p^{12}q^{60}$ 12

1 12 64 200 395 480 288



$p^{12}q^{60}$ 96

1 12 63 190 359 418 245



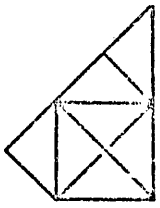
$p^{12}q^{60}$ 32

1 12 63 189 354 411 242

16

$p^{12}q^{60}$

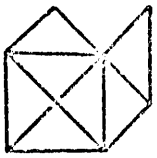
1 12 63 190 357 414 243



144

$p^{12}q^{60}$

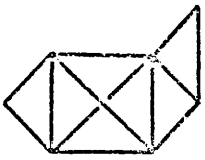
1 12 64 197 378 443 257



144

$p^{12}q^{60}$

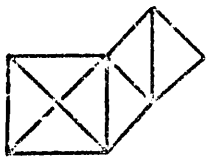
1 12 64 197 378 443 257



96

$p^{12}q^{60}$

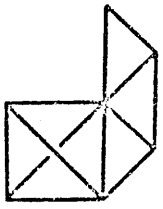
1 12 64 198 383 450 260



96

$p^{12}q^{60}$

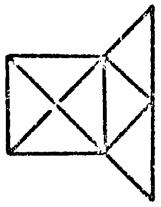
1 12 65 205 402 475 272



96

$p^{12}q^{60}$

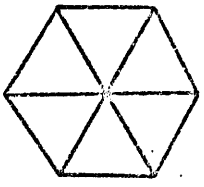
1 12 65 205 402 475 272



24

$p^{12}q^{60}$

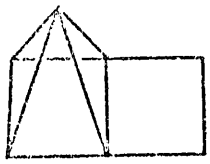
1 12 64 198 383 454 264



16

$p^{12}q^{60}$

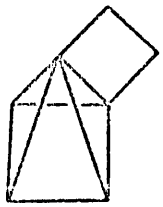
1 12 66 214 435 534 320



24

$p^{11}q^{62}$

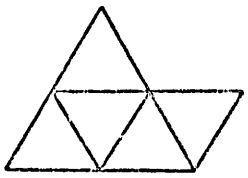
1 11 52 138 213 159



24

$p^{11}q^{62}$

1 11 52 137 209 156



336

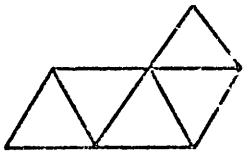
$p^{11}q^{62}$

1 11 52 136 203 141

192

$p^{11}q^{62}$

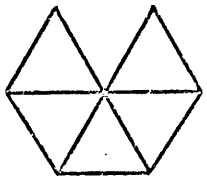
1 11 53 141 210 144



384

$p^{11}q^{62}$

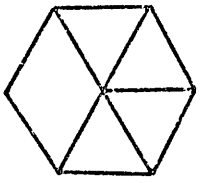
1 11 53 141 210 144



96

$p^{11}q^{62}$

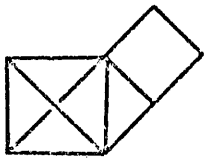
1 11 53 141 210 144



24

$p^{11}q^{62}$

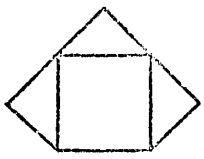
1 11 54 149 235 176



48

$p^{11}q^{62}$

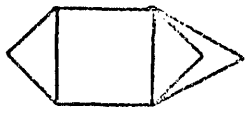
1 11 52 135 201 144



96

$p^{10}q^{64}$

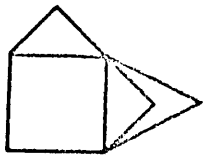
1 10 42 90 81



24

$p^{10}q^{64}$

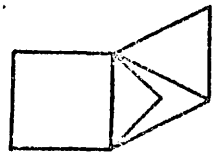
1 10 41 84 76



48

$p^{10}q^{64}$

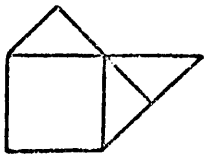
1 10 41 84 76



48

$p^{10}q^{64}$

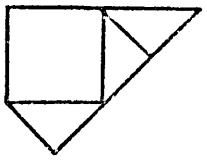
1 10 40 80 73



144

$p^{10}q^{64}$

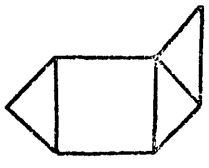
1 10 42 88 79



192

$p^{10}q^{64}$

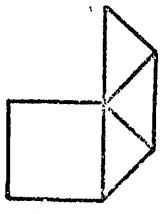
1 10 42 88 79



192

$p^{10}q^{64}$

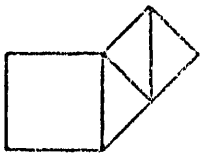
1 10 42 88 79



96

$p^{10}q^{64}$

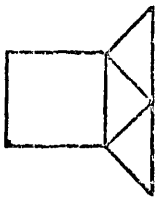
1 10 41 84 76



144

$p^{10}q^{64}$

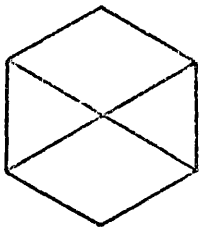
1 10 41 84 76



72

$p^{10}q^{64}$

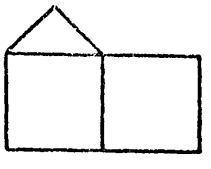
1 10 40 82 75



12

$p^{10}q^{64}$

1 10 43 96 96



48

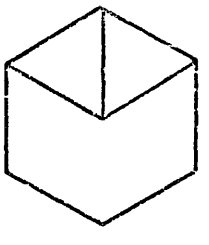
$p^{9}q^{66}$

1 9 31 41

24

$p^{9}q^{66}$

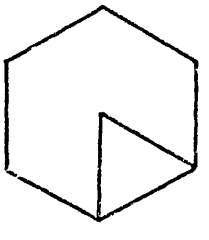
1 9 31 41



24

$p^{9}q^{66}$

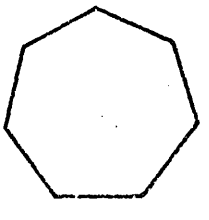
1 9 30 40



360

$p^{8}q^{68}$

1 8 17

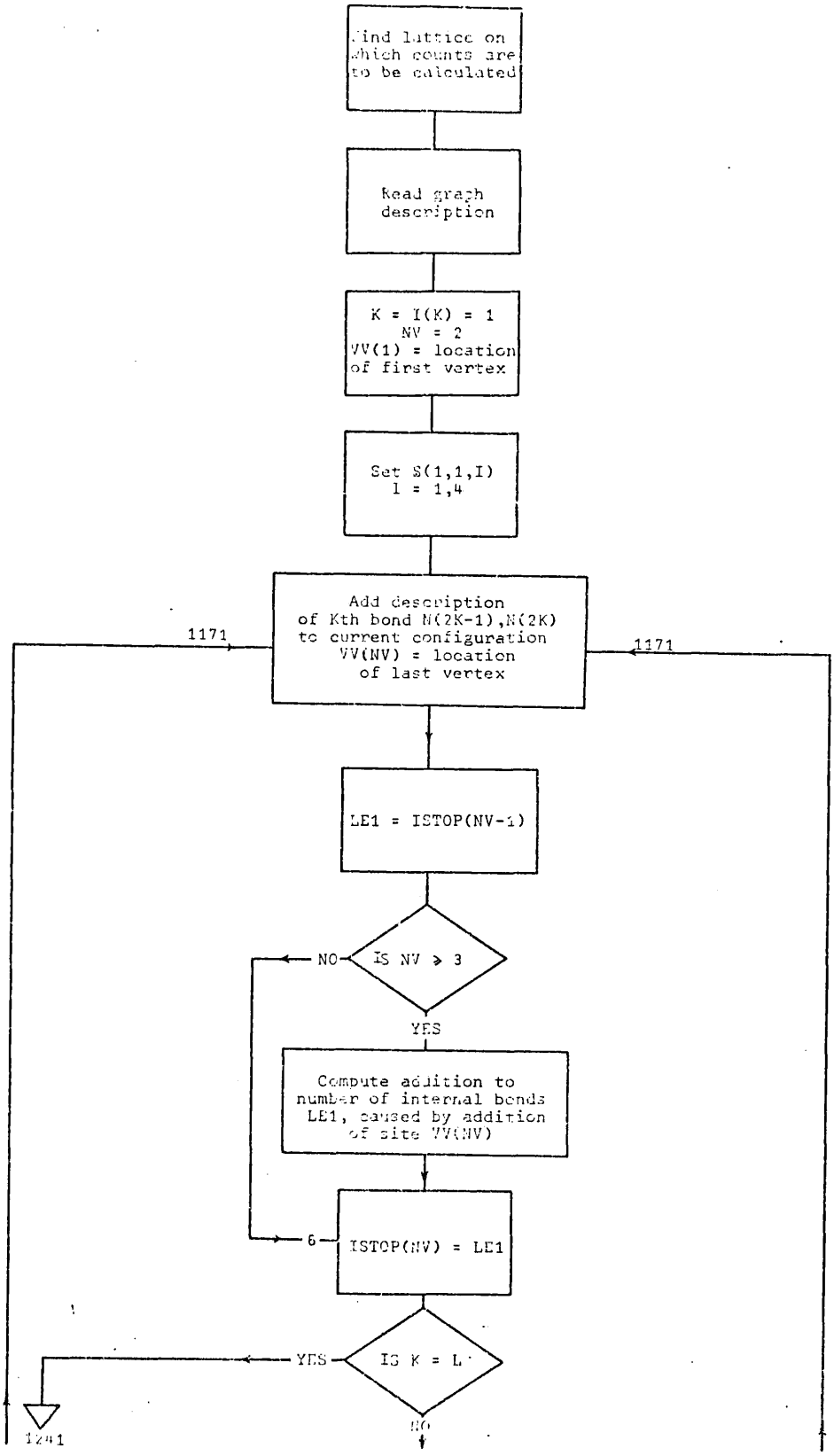


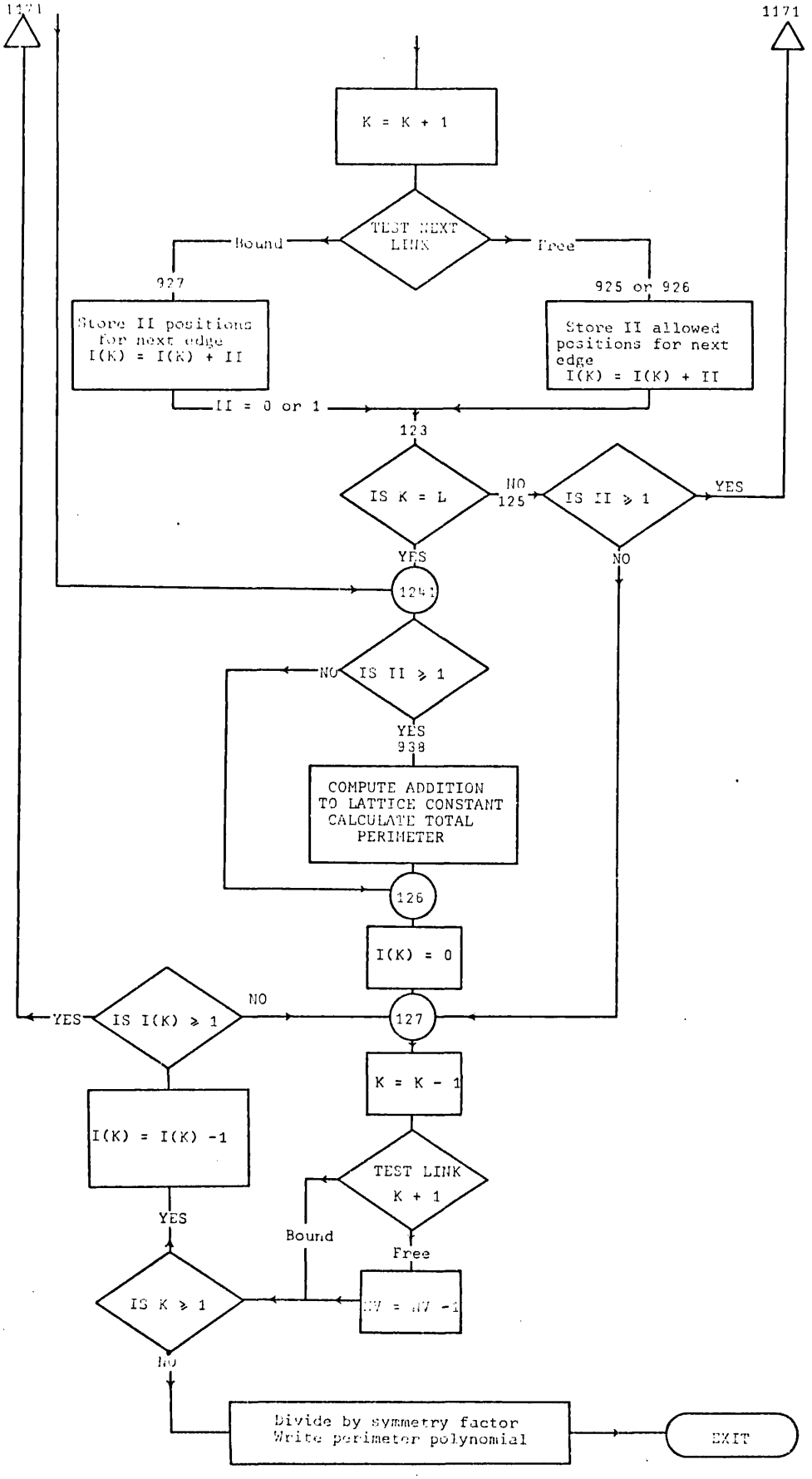
72

$p^{7}q^{70}$

1 7

Flow Chart of CNT2.




1171
1171
K = K + 1
TEST NEXT LINK
Bound
Free
927
925 or 926
Store II positions for next edge I(K) = I(K) + II
Store II allowed positions for next edge I(K) = I(K) + II
II = 0 or 1
123
IS K = L
NO
125
IS II ≥ 1
YES
YES
NO
1241
NO
IS II ≥ 1
YES
938
COMPUTE ADDITION TO LATTICE CONSTANT CALCULATE TOTAL PERIMETER
126
I(K) = 0
YES
IS I(K) ≥ 1
NO
127
K = K - 1
I(K) = I(K) -1
TEST LINK K + 1
YES
Bound
Free
IS K ≥ 1
NV = NV -1
NO
Divide by symmetry factor
Write perimeter polynomial
EXIT

```
JOB(UNAH203,J6,T60,D1,CM30000)
REQUEST (TAPE4,HI)UL0656X*INHIBIT*
FUN(S)
SKIPF(TAPE4,23,15,B)
COPYBF(TAPE4,DISK2)
REWIND(DISK2)
RETURN(TAPE4)
RFL,50000.
LOAD(LGO)
EXECUTE(CNT2,INPUT,OUTPUT,PUNCH,DISK2)
000000000000000000000
       PROGRAM CNT2(INPUT,OUTPUT,PUNCH,TAPE1,TAPE2=INPUT,TAPE3=OUTPUT)
       INTEGER Q,J,IDENT,V,L,TE,A,F,B,X,II,Y,NU,K,XI,NV,HILO
       INTEGER R(12),RBAR(12),T(23),P(100),DEGREE(11)
       INTEGER N(23),S(22,11,4),I(11),THTA(10),ISTOP(9),VV(24),QQ(23)
       INTEGER MWPLUS(50,20),MDLTJ(50,20)MPHI(20),MPHIP(20)
       INTEGER DLTJ(50),WPLUS(50)
       INTEGER PHI,PHIP,WDBAR,NPLUS,JJ,WNEXT
       INTEGER PERM(100),TPERM(100)
       DATA MPHI/6,4,3,12,8,6,4,12,8,18,14,18,18,12,12,42,26,26,2*0/
       DATA MPHIP/4,3,0,5,4,3,14*0/
       DATA MDLTJ/
C      TRIANGULAR
      11,-1,51,52,-51,-52,44*0,
C      SQUARE
      11,-1,51,-51,46*0,
C      HONEYCOMB
      150*0,
C      FCC
      11,-1,51,2601,-2601,-51,2602,2550,2551,-2602,-2550,-2551,38*0,
C      BCC
      11,-1,51,-51,2601,2551,-2601,-2551,42*0,
C      SC
      11,-1,51,-51,2601,-2601,44*0,
      1700*0/
       DATA MWPLUS/
C      TRIANGULAR
      11,1,2,2,46*0,
C      SQUARE
      11,1,2,47*0,
C      HONEYCOMB
      150*0,
C      FCC
      11,1,2,4,4,45*0,
C      BCC
      11,1,3,3,46*0,
C      SC
      11,1,4,47*0,
      1700*0/
       XI=0
10000 CONTINUE
 1002 Q=10
      READ(2,20006)ALATT,HILO
20006 FORMAT (A10,10X,12)
      IF(HILO.EQ.0)GO TO 100
      DO 30 IP=1,100
      TPERM(IP)=0
```

```
   30 PERM(IP)=0
C     PHI IS THE CO-ORDINATION NUMBER
C     PHIP IS THE NUMBER OF WEIGHTED DIRECTIONS.
C     HILO=+1 FOR HIGH TEMPERATURE, -1 FOR LOW TEMPERATURE.
C     THTA CONTAINS THE PAGE HEADING
C     PRINTS THE LAST LINE OF THE PRECEDING LATTICE.
  100 IF(XI-1)10021,901,901
  901 WRITE(3,5000)
      DO 27 IP=1,IM
      IF(TPERM(IP).EQ.0)GO TO 27
      WRITE(3,3000)TPERM(IP),IP
   27 CONTINUE
      XI=0
10021 IF(HILO)4904,903,4904
  903 WRITE(3,20030)
20030 FORMAT (1H1,16HNO MORE LATTICES)
      CALL EXIT
 4904 N=1
      IF(ALATT.EQ.10HTRIANGULAR)GOTO904
      N=N+1
      IF(ALATT.EQ.10HSQUARE)GOTO904
      N=N+1
      IF(ALATT.EQ.10HONEYCOMB)GOTO904
      N=N+1
      IF(ALATT.EQ.10HFCC)GOTO904
      N=N+1
      IF(ALATT.EQ.10HBCC)GOTO904
      N=N+1
      IF(ALATT.EQ.10HSC)GOTO904
      WRITE(3,20050)
20050 FORMAT(1H,22HLATTICE NOT RECOGNISED)
      CALL EXIT
  904 WRITE(3,20008)N(1),ALATT,HILO
20008 FORMAT(1H,I3,2X,A10,10HLATTICE TC,12)
C     DECISION INCREMENTS
C     WPLUS IS THE ARRAY OF WEIGHTS
C     THE TWO DIRECTIONS WITH WEIGHT 1 SHOULD APPEAR FIRST, FOLLOWED BY
C     THE WEIGHTED DIRECTIONS, FOLLOWED BY THE UNWEIGHTED DIRECTIONS
      PHI=MPHI(N)
      PHIP=MPHIP(N)
      DO 4906 J=1,PHI
      DLTJ(J)=MDLTJ(J,N)
 4906 WPLUS(J)=MWPLUS(J,N)
  311 READ(2,20007)IDMIN,IDMAX
      IF(IDMIN)10000,10000,101
  101 READ(1,20001)IDENT,T1,T2,V,L,(T(J),J=1,21),(DEGREE(J),J=1,11)
      DO 1111 I=1,V
 1111 ISTOP(I)=0
      IM=PHI*V
      IDL=2*L
20001 FORMAT(14,A8,A3,2212,17,11I1)
  301 IF(IDENT-IDMIN)101,312,312
  312 IF(IDENT-IDMAX)905,905,311
  905 IF(L-1)906,907,906
  907 TE=PHI
      GOTO131
  906 TE=0
```

```
      DO 908 A=1,L
  908 I(A)=0
      IDUM=2*L
      DO 909 A=1,IDUM
      P(A)=1
  909 N(A)=0
      B=1
      P(1)=3
  116 B=B+1
      IF(B-L)113,113,117
  113 A=2*B
      IF(T(A))910,116,910
  910 P(B)=P(B)+2
      GOTO116
  117 IF(HILO)837,837,829
  837 DO871 J=1,L
  871 QQ(J)=0
      B=0
  827 B=B+1
      IF(B-L)828,829,829
  828 A=2*B
      IF(P(B)-2)830,831,827
  830 X=A
      GOTO832
  831 X=A-1
  832 J=B
  833 J=J+1
      IF(J-L)981,981,827
  981 IF(P(J)-2)833,833,834
  834 JJ=2*J
      IF(X-T(JJ-1))833,982,835
  835 IF(X-T(JJ))833,836,833
  982 IF(X-T(JJ))833,836,836
  836 QQ(B)=QQ(B)+1
      GOTO833
  829 K=1
      I(K)=1
      IDUM=I(K)
      VV(1)=61226
      VV(2)=61226+DLTJ(1)
      NV=2
      S(IDUM,K,1)=61226
      S(IDUM,K,2)=61226+DLTJ(1)
      S(IDUM,K,3)=PHI
      S(IDUM,K,4)=1
C     S(A,B,3) IS THE WEIGHT IF A,B IS USED
C     S(A,B,4) IS 1 IF WEIGHTS ARE TO BE USED FOR NEXT LINE
 1171 NU=2*K
C     N(J)CONTAINS DESCRIPTION OF CONFIGURATION SO FAR.
C     ADD LAST BOND OF COLUMN K TO CONFIGURATION DESCRIPTION AND
C     DECIDE ON WEIGHTS
      IDUM=I(K)
      N(NU-1)=S(IDUM,K,1)
      N(NU)=S(IDUM,K,2)
      WDBAR=S(IDUM,K,3)
      WNEXT=S(IDUM,K,4)
      IF (P(K)-2)960,961,962
```

```
  960  VV(NV)=S(IDUM,K,2)
       GOTO962
  961  VV(NV)=S(IDUM,K,1)
  962  IF(WNEXT-1)921,922,921
  922  NPLUS=PHIP
       GOTO 1172
  921  NPLUS=PHI
 1172  CONTINUE
       LE1=ISTOP(NV-1)
       IF(NV.LT.3)GO TO 6
       LE=VV(NV)
       IX=1
    5  L1=LE+DLTJ(IX)
       J=NV-1
    3  IF(L1-VV(J))1,2,1
    2  M1=2*K
   11  IF(M1.LE.0)GO TO 14
       IF(LE.EQ.N(M1))GO TO 10
   15  M1=M1-2
       GO TO 11
   10  IF(L1-N(M1-1))15,1,15
   14  LE1=LE1+1
    1  J=J-1
       IF(J.EQ.0)GO TO 4
       GO TO 3
    4  IX=IX+1
       IF(IX-PHI)5,5,6
    6  ISTOP(NV)=LE1
  118  IF(K-L+1)923,923,1241
  923  K=K+1
       NU=2*K
       II=0
       I3=WDBAR*WNEXT
       I4=WDBAR-I3
C      SELECT TYPE OF LINK
       IF(P(K)-2)926,925,927
C      START SEARCH FOR A BOUND-FREE LINK
  925  IDUM=I(NU)
       JJ=N(IDUM)
       GOTO119
  926  IDUM=T(NU-1)
       JJ=N(IDUM)
  119  Y=0
       NV=NV+1
       I1=P(K)
       I2=3-P(K)
  120  Y=Y+1
       IF(Y-NPLUS)928,928,123
  928  X=JJ+DLTJ(Y)
       A=0
  121  A=A+1
       IF(A-NV+1)929,929,122
  929  IF(VV(A)-X)121,120,121
  122  IF(HILO)971,971,970
  971  IDUM=0
       A=0
  965  A=A+1
```

```
      IF(A-NV+1)966,966,967
  966 DO968 J=1,PHI
      IF(VV(A)+DLTJ(J)-X)968,969,968
  968 CONTINUE
      GOTO965
  969 IDUM=IDUM+1
      GOTO 965
  967 IF(QQ(K)-IDUM+1)120,970,120
  970 II=II+1
C       ARE WEIGHTS NEEDED NEXT TIME
      S(II,K,3)=I4+I3*WPLUS(Y)
      IF(Y-2)930,930,931
  930 S(II,K,4)=WNEXT
      GOTO1221
  931 S(II,K,4)=0
C     STORE BOND LOCATION
 1221 S(II,K,I1)=JJ
      S(II,K,I2)=X
      GO TO 120
C     START SEARCH FOR BOUND-BOUND LINK
  927 IDUM=T(NU-1)
      JJ=N(IDUM)
  129 Y=0
  130 Y=Y+1
      IF(Y-NPLUS)943,943,123
  943 X=JJ+DLTJ(Y)
      IDUM=T(NU)
      IF(X-N(IDUM))130,944,130
  944 II=II+1
C       ARE WEIGHTS NEEDED NEXT TIME
      S(II,K,3)=I4+I3*WPLUS(Y)
      IF(Y-2)945,945,946
  945 S(II,K,4)=WNEXT
      GO TO 1301
  946 S(II,K,4)=0
C     STORE BOND LOCATION
 1301 S(II,K,1)=JJ
      S(II,K,2)=X
      GO TO 130
C     CHECK IF LAST LINK
  123 I(K)=II
      IF(K-L)125,1241,936
  936 X=23
      GO TO 139
  125 IF(II-1)127,1171,1171
 1241 IF(II-1)126,938,938
C     COMPUTE ADDITION TO LATTICE CONSTANT
  938 IDUM=I(K)
      DO 940 II=1,IDUM
      LTE=0
      LTE=S(II,K,3)
      TE=TE+LTE
      VV(V)=S(II,K,2)
      N(IDL)=VV(V)
      N(IDL-1)=S(II,K,1)
      LE1=ISTOP(V-1)
   22 LE=VV(V)
```

```
      IX=1
   20 L1=LE+DLTJ(IX)
      J=V-1
   18 IF(L1-VV(J))16,17,16
   17 M1=2*K
   24 IF(M1.LE.0)GO TO 25
      IF(LE.EQ.N(M1))GO TO 23
   26 M1=M1-2
      GO TO 24
   23 IF(L1-N(M1-1))26,16,26
   25 LE1=LE1+1
   16 J=J-1
      IF(J.EQ.0)GO TO 19
      GO TO 18
   19 IX=IX+1
      IF(IX-PHI)20,20,8
    8 LE1=PHI* V-2*L -LE1
        PERM(LE1)=PERM(LE1)+LTE
  940 CONTINUE
  126 I(K)=0
  127 K=K-1
      IF(K(K+1)-2)963,963,964
  963 NV=NV-1
C     HAS THE LAST POSSIBILITY BEEN TRIED
  964 IF(K-1)131,941,941
  941 I(K)=I(K)-1
      IF(I(K)-1)127,1171,1171
  131 TE=TE/T(21)
      WRITE(3,4000)IDENT,TE
      DO 31 IP=1,IM
      IF(PERM(IP).EQ.0)GO TO 31
      TPERM(IP)=TPERM(IP)+PERM(IP)/T(21)
      PERM(IP)=PERM(IP)/T(21)
      WRITE(3,5001)PERM(IP),IP
      PERM(IP)=0
   31 CONTINUE
      Q=2*L
      IF(TE-1)101,949,949
  949 XI=XI+1
      GO TO 101
  199 WRITE(3,20009)X
      GO TO 101
 3000 FORMAT(*COUNT=*,I10,5X,*PERIMETER=*,I10)
 4000 FORMAT(//,*GRAPH IDENTITY*,I10,5X,*TOTAL COUNT*,I10)
 5001 FORMAT(/,2X,*PARTIAL COUNT*,I10,2X,*PERIMETER*,I10)
 5000 FORMAT(/,*THE COMPLETE PERIMETER PLYNOMIAL FOR THE ABOVE GRAPHS
     1ON THIS LATTICE IS*)
20007 FORMAT(12I5)
20009 FORMAT(1HQ,8HERROR NO, I6)
20016 FORMAT(5(I4,I10))
20017 FORMAT(1H,5(I4,I10,10X))
      END
```

Appendix V

Graph Definitions

1. An *articulation point* or *cut-vertex* is a vertex of a connected graph, the deletion of which produces a graph which is not connected.

2. The *deletion of a vertex* i from any graph G means the removal of the vertex i from the vertex set of G and the removal of all incident edges from the edge set of G.

3. The *bond closure* $\overline{E'}$ of a subset E' of the edge set E of a graph $G = (V,E)$ is the set of all edges of E which have both terminal vertices in the same component of $G' = (V,E')$. A subset for which $\overline{E'} = E'$ is said to be *bond closed* in G.

4. The *decoration* or *completion of a simple face* of $n > 2$ vertices of an undirected plane graph is the addition of $\frac{1}{2}n(n-3)$ new edges constructed by drawing, within the face, all possible diagonal lines. This converts the face with its boundary edges to a complete graph $K(n)$ drawn with crossing lines which is termed a *multiface* in distinction to an *ordinary face*.

5. The *matching graph* G^M of a simple semiplanar graph G is obtained from the underlying graph G_o by completing all those faces of G_o not completed in G.

6. The *weak k-weight* of a graph G is defined recursively by

$$k(G) = n(G) - \sum_{G'} k(G')$$

where $n(G)$ is the number of components of G , and the sum runs over all proper subgraphs, G' , of G .

7. The *strong K-weight* of a graph G is defined recursively by

$$K(G) = n(G) - \sum_{G^*} K(G^*)$$

where $n(G)$ is the number of components of G , and the sum runs over all proper section graphs, G* , of G .

8. A *subgraph* G' of a graph G is a graph obtained from G by deleting a subset (which may be null sets) of its vertices and edges.

The *covering graph* G^C *of an undirected graph* G is constructed as follows: (a) with each edge of G is associated a new vertex; these new vertices constitute the vertex set of G^C ; (b) any two distinct vertices of G^C corresponding to *adjacent edges* of G are connected by a single edge of G^C .

Appendix VI

Variation of $\bar{w}$ with s .

If we fit $\nu_s = \dfrac{\bar{w}_s}{\bar{w}_{s-1}}$ to a curve of the form $1 + A/s + B/s^2$ then if $\bar{w}_s \underset{s\to\infty}{\sim} s$ we expect A to have a value one and the intercept of ν_s plotted against $1/s$ to be one.

In the following tables $\bar{w}_s$, ν_s , A and the successive intercepts $I_n = s\bar{w}_s - (s-1)\bar{w}_{s-1}$ are recorded for various two and three dimensional lattices.

Simple Quadratic Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	7.333	1.222	-	0.0
4	8.632	1.177	1.0415	0.833
5	9.905	1.148	1.0294	0.855
6	11.167	1.127	1.0269	0.899
7	12.416	1.112	1.0186	0.895
8	13.653	1.100	1.0143	0.897
9	14.883	1.090	1.0131	0.916
10	16.107	1.082	1.0119	0.928
11	17.326	1.076	1.0104	0.937
12	18.541	1.070	1.0092	0.944
13	19.754	1.065	1.0084	0.951

Triangular Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	9.818	1.227	-	0.712
4	11.591	1.181	1.0404	0.843
5	13.323	1.149	1.0248	0.846
6	15.031	1.128	1.0223	0.881
7	16.722	1.113	1.0183	0.897
8	18.401	1.100	1.0156	0.912
9	20.070	1.091	1.0135	0.924

Simple Quadratic Matching Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	13.800	1.255	-	0.791
4	16.482	1.194	1.0137	0.818
5	19.110	1.159	1.0199	0.877
6	21.704	1.136	1.0172	0.900
7	24.274	1.118	1.0147	0.917

Hexagonal Matching Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	20.818	1.262	-	0.855
4	25.021	1.202	1.0227	0.876
5	29.154	1.165	1.0176	0.896
6	33.237	1.140	1.0149	0.915
7	37.287	1.122	1.0125	0.928

Simple Cubic Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	13.200	1.320	-	0.213
4	16.256	1.232	0.9660	0.824
5	19.213	1.182	0.9838	0.845
6	22.129	1.152	1.0006	0.914
7	25.018	1.131	1.0036	0.936
8	27.890	1.115	1.0044	0.949
9	30.749	1.103	1.0043	0.957

Simple Cubic with 1st, 2nd and 3rd neighbours

s	$\bar{w}_s$	ν_s	I_s	A_s
3	52.987	1.330	-	0.838
4	65.724	1.240	0.9721	0.878
5	78.251	1.191	0.9915	0.919
6	90.647	1.158	0.9975	0.938

Body Centred Cubic Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	18.286	1.306	-	-
4	22.500	1.230	1.0035	0.932
5	26.654	1.185	1.0012	0.928
6	30.769	1.154	1.0034	0.943
7	34.854	1.133	1.0031	0.948

Face Centred Cubic Lattice

s	$\bar{w}_s$	ν_s	I_s	A_s
3	23.440	1.302	-	0.720
4	28.737	1.226	0.9972	0.896
5	33.956	1.182	1.0042	0.925
6	39.121	1.152	1.0046	0.936
7	44.247	1.131	1.0046	0.944

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