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Percolation processes in d -dimensions

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Abstract. Series data for the mean cluster size for site mixtures on a d -dimensional simple hypercubical lattice are presented. Numerical evidence for the existence of a critical dimension for the cluster growth function and for the mean cluster size is examined and it is concluded that $d_c = 6$.

Exact expansions for the mean number of clusters $K(p)$ and the mean cluster size $S(p)$ in powers of $1/\sigma$ where $\sigma = 2d - 1$ and $p < p_c$ are derived through fifth and third order, respectively. The zeroth-order terms are the Bethe approximations.

The growth parameter λ is found to have the expansion

$$\lambda = \lambda_B(1 - \frac{1}{2}\sigma^{-1} - 2\sigma^{-2} - \dots)$$

where λ_B is the value of λ in the Bethe approximation. Similarly the critical probability p_c can be expanded in inverse powers of σ as

$$p_c = \sigma^{-1} + \frac{1}{2}\sigma^{-2} + \frac{3}{4}\sigma^{-3} + \frac{20}{4}\sigma^{-4} + \dots$$

Although these expansions are probably only asymptotic, they yield good approximations even when $d = 3$.

1. Introduction

Hyperdimensional lattices have recently been studied by many authors (Thompson 1974, Thompson and Gates 1974, Baker 1974, 1975, Gerber and Fisher 1974, 1975). It has been conjectured (Toulouse 1974) that the critical dimension for percolation is $d_c = 6$, instead of the $d_c = 4$ found for second-order phase transitions (with short range interactions); above this the critical exponents should be classical and dimension independent. (For a general introduction see Toulouse and Pfeuty 1975.) It has been suggested that this conjecture might be tested by numerical studies (Toulouse 1974, Domb, private communication). In this paper we present series expansion data for the d -dimensional cubic lattice and draw some tentative conclusions from their analysis. Kirkpatrick (1976) has also studied the problem but using Monte Carlo methods.

The general techniques available for series development in higher dimensions have been described in detail by Fisher and Gaunt (1964) in their study of the Ising and excluded volume problems on a d -dimensional cubic lattice; the derivation of low density series expansions for a study of percolation processes has been described by Sykes and Glen (1976). By combining the methods described by these authors we have derived data for the *site* percolation problem on a d -dimensional cubic lattice. Since no new elements are introduced into the calculation we simply summarize the results in § 2.

For the percolation problem we have confined our study to the critical exponent γ for the mean size defined as usual by

$$S(p) \approx C(p_c - p)^{-\gamma}, \quad p \rightarrow p_c \quad (1.1)$$

since this has been found to be the exponent most accessible by series methods in two and three dimensions (Sykes *et al* 1976a, b, c, d). (For a definition of $S(p)$ see Sykes and Glen 1976.) The dimension independent limit for $d > d_c$ in (1.1) is $\gamma = 1$; this is the value found for the Bethe approximation. (We give $S_B(p)$ explicitly in (3.17).)

We also study the asymptotic behaviour of the total number, N_s , of connected clusters of s sites. This defines a critical exponent θ through

$$N_s \approx A s^{-\theta} \lambda^s, \quad s \rightarrow \infty. \quad (1.2)$$

The form (1.2) has been studied in two and three dimensions by Sykes and Glen (1976) and Sykes *et al* (1976d). The amplitude A and the growth parameter λ are known exactly for the Bethe approximation (we give them explicitly in (3.8) and (3.9)) and the corresponding dimension independent limit is $\theta = 2\frac{1}{2}$.

On general grounds it is usually supposed that the Bethe approximation will become more accurate with increasing coordination number ν and we have used the general techniques introduced by Fisher and Gaunt (1964) to derive expansions in $1/\sigma$, where $\sigma = 2d - 1 = \nu - 1$, which correspond effectively to developments in inverse powers of the dimension. These developments serve as a useful alternative to supplement the direct expansions in high dimensions.

2. Series expansions

We have derived the first seven *perimeter polynomials* for the simple hypercubical lattice system studied by Fisher and Gaunt (1964 § 2). These are a straightforward generalization of those defined by Sykes and Glen (1976) § 2. Denoting as usual the respective expectations of the two species of site by p and q and the dimension of the lattice by d we find:

$$D_1(d) = q^{2d}$$

$$D_2(d) = q^{4d-2} \binom{d}{1}$$

$$D_3(d) = q^{6d-4} \left[\binom{d}{1} + 4q^{-1} \binom{d}{2} \right]$$

$$D_4(d) = q^{8d-6} \left[\binom{d}{1} + (8q^{-1} + 9q^{-2}) \binom{d}{2} + (24q^{-2} + 8q^{-3}) \binom{d}{3} \right]$$

$$D_5(d) = q^{10d-8} \left[\binom{d}{1} + (12q^{-1} + 28q^{-2} + 20q^{-3} + q^{-4}) \binom{d}{2} \right. \\ \left. + (72q^{-2} + 168q^{-3} + 96q^{-4} + 12q^{-5}) \binom{d}{3} + (192q^{-3} + 192q^{-4} + 16q^{-6}) \binom{d}{4} \right]$$

$$D_6(d) = q^{12d-10} \left[\binom{d}{1} + (16q^{-1} + 60q^{-2} + 80q^{-3} + 54q^{-4} + 4q^{-5}) \binom{d}{2} \right. \\ \left. + (144q^{-2} + 720q^{-3} + 966q^{-4} + 720q^{-5} + 280q^{-6} + 6q^{-8}) \binom{d}{3} \right. \\ \left. + (768q^{-3} + 3264q^{-4} + 2784q^{-5} + 1504q^{-6} + 288q^{-7} + 32q^{-9}) \binom{d}{4} \right. \\ \left. + (1920q^{-4} + 3840q^{-5} + 480q^{-6} + 640q^{-7} + 32q^{-10}) \binom{d}{5} \right]$$

$$\begin{aligned}
 D_7(d) = & q^{14d-12} [\binom{d}{1} + (20q^{-1} + 100q^{-2} + 228q^{-3} + 252q^{-4} + 136q^{-5} + 22q^{-6}) \binom{d}{2} \\
 & + (240q^{-2} + 1880q^{-3} + 4926q^{-4} + 6024q^{-5} + 4924q^{-6} + 2496q^{-7} \\
 & + 662q^{-8} + 72q^{-9} + q^{-12}) \binom{d}{3} + (1920q^{-3} + 15744q^{-4} + 36624q^{-5} \\
 & + 36256q^{-6} + 25440q^{-7} + 10320q^{-8} + 2288q^{-9} + 672q^{-10} + 24q^{-13}) \binom{d}{4} \\
 & + (9600q^{-4} + 63360q^{-5} + 89760q^{-6} + 57920q^{-7} + 23680q^{-8} \\
 & + 7680q^{-9} + 1760q^{-10} + 960q^{-11} + 80q^{-14}) \binom{d}{5} + (23040q^{-5} + 76800q^{-6} \\
 & + 28800q^{-7} + 19200q^{-8} + 3840q^{-9} + 1920q^{-11} + 64q^{-15}) \binom{d}{6}]. \tag{2.1}
 \end{aligned}$$

We have also derived the expansion for the mean number of clusters in general form through p^{11} :

$$\begin{aligned}
 K_d(p) = & p - \binom{d}{1} p^2 + \binom{d}{2} p^4 + 4 \binom{d}{3} p^6 - 8 \binom{d}{3} p^7 + [\binom{d}{2} + 27 \binom{d}{3} + 168 \binom{d}{4}] p^8 \\
 & - [\binom{d}{2} + 72 \binom{d}{3} + 720 \binom{d}{4}] p^9 + [2 \binom{d}{2} + 318 \binom{d}{3} + 4544 \binom{d}{4} + 12096 \binom{d}{5}] p^{10} \\
 & - [4 \binom{d}{2} + 1032 \binom{d}{3} + 19648 \binom{d}{4} + \dots \binom{d}{5}] p^{11} + \dots \tag{2.2}
 \end{aligned}$$

Using the general expansion and manipulative procedures described by Sykes and Glen (1976) § 2 we obtain from (2.1) and the first nine coefficients of (2.2) the total number of clusters with s -sites, N_s , through N_9 for all d . We give the explicit values for

Table 1. Total number of clusters (N_s) of s sites on a d -dimensional cubic lattice.

	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$
N_1	1	1	1	1	1	1
N_2	2	3	4	5	6	7
N_3	6	15	28	45	66	91
N_4	19	86	234	495	901	1 484
N_5	63	534	2 162	6 095	13 881	27 468
N_6	216	3 481	21 272	80 617	231 008	551 313
N_7	760	23 502	218 740	1 121 075	4 057 660	11 710 328
N_8	2 725	162 913	2 323 730	16 177 405	74 174 927	259 379 101
N_9	9 910	1 152 870	25 314 097	240 196 280	1 398 295 989	5 933 702 467
N_{10}	36 446	8 294 738	281 345 096	3 648 115 531		
N_{11}	135 268	60 494 549	3 178 474 308			
N_{12}	505 861	446 205 905				
N_{13}	1 903 890	3 322 769 129				
N_{14}	7 204 874					
N_{15}	27 394 666					
N_{16}	104 592 937					
N_{17}	400 795 844					
N_{18}	1 540 820 542					
N_{19}	5 940 738 676					

$d = 2, 3, 4, 5, 6$ and 7 in table 1 since these are the numbers we study numerically. In 3, 4 and 5 dimensions we have extended the data by deriving extra perimeter polynomials and extra coefficients in the mean number expansion; the data for $d = 2$ is taken from Sykes and Glen (1976).

Alternatively the data can be summarized for all dimensions in the form

$$N_s(d) = \sum_{\xi=1}^{s-1} A_{\xi}^s \binom{d}{s-\xi} \tag{2.3}$$

$$= 2^{s-1} s^{s-3} \binom{d}{s-1} + 2^{s-3} s^{s-5} (s-2)(2s^2-6s+9) \binom{d}{s-2} + 2^{s-5} s^{s-7} (s-3) \times \frac{(12s^5 - 104s^4 + 360s^3 - 679s^2 + 1122s - 1560)}{6} \binom{d}{s-3} + \dots \tag{2.4}$$

$(s \geq 3).$

The calculation of successive A_{ξ}^s numerically for values of s through $s = 9$ is a matter of arithmetic; the calculation of the A_{ξ}^s as functions of s is difficult. Contributions to A_1^s come from Cayley trees since these are the only clusters which can enter all dimensions; hence the first term of (2.4) follows from the rigorous result of Fisher and Essam (1961), equation (14). The second and third terms are confirmed by the data of table 1. The form of (2.4) is not in agreement with the results of Lunnon (1974) whose values for A_1^6 and A_2^6 would seem to be in error.

We have obtained the expansion for the mean cluster size

$$S(p) = \sum_r b_r p^r \tag{2.5}$$

for all d through b_8 and we have supplemented the data for $d = 2, 3, 4$ and 5 as aforementioned. We tabulate the coefficients in table 2. Here again the data can be

Table 2. Coefficients for expansion of $S(p) = \sum_r b_r p^r$ on a d -dimensional cubic lattice.

	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$
b_1	4	6	8	10	12	14
b_2	12	30	56	90	132	182
b_3	24	114	320	690	1 272	2 114
b_4	52	438	1 832	5 290	12 252	24 542
b_5	108	1 542	9 944	39 210	115 332	280 238
b_6	224	5 754	55 184	293 570	1 091 472	3 210 074
b_7	412	19 574	290 104	2 135 370	10 159 252	36 394 302
b_8	844	71 958	1 596 952	15 839 690	95 435 172	414 610 014
b_9	1 528	233 574	8 237 616	113 998 170		
b_{10}	3 152	870 666	45 100 208			
b_{11}	5 036	2 696 274				
b_{12}	11 984	10 373 274				
b_{13}	15 040					
b_{14}	46 512					
b_{15}	34 788					
b_{16}	197 612					
b_{17}	4 036					
b_{18}	929 368					

summarized in the alternative form

$$b_r(d) = \sum_{\xi=0}^{r-1} B_{\xi}^r \binom{d}{r-\xi} \tag{2.6}$$

$$\begin{aligned} &= 2^r r! \binom{d}{r} + 2^{r-2} (r-1)! (2r^2 - 7r + 8) \binom{d}{r-1} \\ &\quad + 2^{r-4} (r-2)! \frac{12r^4 - 116r^3 + 435r^2 - 799r + 732}{6} \binom{d}{r-2} + 2^{r-6} (r-3)! \\ &\quad \times \frac{8r^6 - 148r^5 + 1142r^4 - 4805r^3 + 12125r^2 - 18960r + 17796}{6} \\ &\quad \times \binom{d}{r-3} + \dots \quad (r \geq 6) \end{aligned} \tag{2.7}$$

where the numerical calculation of successive B_{ξ}^r through $r = 8$ is a matter of arithmetic and the derivation of the more general form is difficult.

By further effort it should be possible to add one or two more terms to the series derived, in most cases, but in the light of our conclusions in § 4 we have not thought this worthwhile at present.

3. Expansions in $1/\sigma$

By following the general methods developed by Fisher and Gaunt (1964) we now derive expansions in the variable $1/\sigma$ where $\sigma = \nu - 1 = 2d - 1$, ν being the coordination number of the lattice. This is facilitated by first expressing the binomial coefficient $\binom{d}{s}$ in inverse powers of σ ; we find

$$\binom{d}{s} = \frac{1}{2^s s!} \prod_{k=0}^{s-1} (\sigma - (2k - 1)) \tag{3.1}$$

$$\begin{aligned} &= (\sigma^s / 2^s s!) [1 - s(s-2)\sigma^{-1} + \frac{1}{6}s(s-1)(3s^2 - 13s + 11)\sigma^{-2} \\ &\quad - \frac{1}{6}s(s-1)(s-2)^2(s^2 - 5s + 3)\sigma^{-3} + \dots] \end{aligned} \tag{3.2}$$

Substituting (3.2) into (2.4) gives

$$\begin{aligned} N_s(d) &= \frac{s^{s-3}}{(s-1)!} \sigma^{s-1} \left(1 - \frac{(s-1)(4s^2 - 21s + 18)}{2s^2} \sigma^{-1} \right. \\ &\quad \left. + \frac{(s-1)(s-2)(48s^4 - 535s^3 + 2295s^2 - 4926s + 4680)}{24s^4} \sigma^{-2} - \dots \right) \end{aligned} \tag{3.3}$$

$(s \geq 3).$

If formally we take the logarithm of this expression we find

$$\begin{aligned} \ln N_s(d) &= (s-1) \ln \sigma - \frac{s}{2} \ln s + s - \frac{1}{2} \ln 2\pi - \sum_{m=1}^{\infty} \frac{B_{2m}}{2m(2m-1)s^{2m-1}} \\ &\quad - \frac{(s-1)(4s^2 - 21s + 18)}{2s^2} \sigma^{-1} \\ &\quad - \frac{(s-1)(79s^4 - 1106s^3 + 5493s^2 - 11292s + 8388)}{24s^4} \sigma^{-2} - \dots \end{aligned} \tag{3.4}$$

where the B_n are Bernoulli numbers and we have used Stirling's formula for $\ln(s-1)!$. We may now use the definition (1.2)

$$\ln \lambda(d) = \lim_{s \rightarrow \infty} \frac{1}{s} \ln N_s(d) \quad (3.5)$$

to derive an expansion in powers of $1/\sigma$ for the limit λ ; thus,

$$\ln \lambda(d) = \ln \sigma + 1 - 2\sigma^{-1} - 3\frac{7}{24}\sigma^{-2} - \dots \quad (3.6)$$

which will continue in this way provided, as seems probable, that the higher coefficients of (3.4) are also of $O(s)$ for s large. Using the rigorous results of Fisher and Essam (1961) it can be shown that in the Bethe approximation the total number of clusters with s -sites is given asymptotically by

$$N_s = A s^{-5/2} [\sigma^\sigma / (\sigma-1)^{\sigma-1}]^s \quad (s \rightarrow \infty) \quad (3.7)$$

where the amplitude

$$A = (\sigma/2\pi)^{1/2} (\sigma+1)(\sigma-1)^{-5/2}. \quad (3.8)$$

Thus, in the Bethe approximation the growth parameter λ is given by

$$\lambda_B = \sigma^\sigma / (\sigma-1)^{\sigma-1}. \quad (3.9)$$

From (3.6) and (3.9) we find

$$\ln(\lambda/\lambda_B) = -\frac{1}{2}\sigma^{-1} - 3\frac{1}{8}\sigma^{-2} - \dots \quad (3.10)$$

or, taking exponentials,

$$\lambda = \lambda_B (1 - \frac{1}{2}\sigma^{-1} - 2\sigma^{-2} - \dots). \quad (3.11)$$

This expansion is the analogue of the $1/\sigma$ -expansions derived by Fisher and Gaunt for the excluded volume limit and the Ising critical point (see Fisher and Gaunt (1964) equations (5.18*b*) and (5.28*b*)). Like those expansions, (3.11) is probably asymptotic. Certainly for the spherical model the corresponding expansion for the critical temperature T_c can be shown rigorously to be only asymptotic (Gerber and Fisher 1974). Unlike the expansions of Fisher and Gaunt where the first-order correction term to the Bethe approximation is of second-order in $(1/\sigma)$, the leading correction term in (3.11) is of first-order.

If (3.11) is asymptotic, then truncation at the smallest term for given σ should yield the optimum approximation. Unfortunately the expansion is so short that it is impossible to tell if the smallest term has been attained in any dimension. Consequently we have estimated λ by truncation after the last term in all cases. These values, $\lambda^{(\sigma)}$, are compared in table 3 with the best series estimates obtained in the next section. Not surprisingly the $1/\sigma$ expansion is not very accurate for $d=2$, but by $d=3$ $\lambda^{(\sigma)}$ is already only 9.4% too small. For $d=4, 5$ and 6 values of $\lambda^{(\sigma)}$ fall within the numerical uncertainties of the series estimates and are only 1.5%, 0.68% and 0.95% smaller than the central estimates, respectively.

A similar procedure can be followed for the coefficients $b_r(d)$ of the mean cluster size (2.5). Thus substituting (3.1) into (2.7) we find

$$b_r(d) = \sigma^r [1 - (\frac{1}{2}r - 4)\sigma^{-1} + (\frac{1}{8}r^2 - 8\frac{5}{8}r + 18\frac{1}{2})\sigma^{-2} - (\frac{9}{16}r^3 - 8\frac{7}{16}r^2 + 54\frac{1}{2}r - 162\frac{3}{4})\sigma^{-3} + \dots], \quad (r \geq 6) \quad (3.12)$$

Table 3. Estimates for critical parameters.

d	2	3	4	5	6
$p_c(d)$	0.593 ± 0.002	0.310 ± 0.004	0.197 ± 0.006	0.141 ± 0.003	0.108 ± 0.003
$p_c^{(\sigma)}(d)$	0.7315	0.31	0.1988	0.1400	0.1085
$p_c^{(MC)}(d)$		0.312 ± 0.001	0.198 ± 0.001	0.141 ± 0.001	0.106 ± 0.001
$\gamma(d)$	2.43 ± 0.03	1.66 ± 0.07	1.41 ± 0.25	1.25 ± 0.15	1.06 ± 0.20
$\gamma^{(MC)}(d)$	2.3 ± 0.1	1.80 ± 0.05	1.6 ± 0.1	1.3 ± 0.1	1.0 ± 0.05
$\lambda(d)$	4.06 ± 0.02	8.35 ± 0.04	13.35 ± 0.2	18.8 ± 0.4	24.4 ± 0.9
$\lambda^{(\sigma)}(d)$	1.875	7.568	13.148	18.673	24.169
$\theta(d)$	1.00 ± 0.05	1.50 ± 0.09	1.90 ± 0.15	2.25 ± 0.30	2.5 ± 0.4

where the coefficient of σ^{-m} is a polynomial in r of degree m . The structure of (3.12) is considerably simpler than that of (3.3) and taking the logarithm yields

$$\ln b_r(d) = r \ln \sigma - (1\frac{1}{2}r - 4)\sigma^{-1} - (2\frac{5}{8}r - 10\frac{1}{2})\sigma^{-2} - (16\frac{1}{4}r - 110\frac{1}{12})\sigma^{-3} - \dots \quad (3.13)$$

Remarkably the terms in r^2, r^3, \dots have cancelled identically and assuming, as seems probable, that this cancellation will continue in the general m th term, the logarithm will be formally linear in r to all orders. This simple situation also obtains for the excluded volume and Ising limits (Fisher and Gaunt 1964, equations (5.16) and (5.27)), in contrast to the more complicated behaviour of (3.4) where, as previously mentioned, the general term is only asymptotically linear in s . If, following (3.5), we formally define a limit μ by

$$\ln \mu(d) = \lim_{r \rightarrow \infty} \frac{1}{r} \ln b_r(d) \quad (3.14)$$

then we find

$$\ln \mu(d) = \ln \sigma - 1\frac{1}{2}\sigma^{-1} - 2\frac{5}{8}\sigma^{-2} - 16\frac{1}{4}\sigma^{-3} - \dots \quad (3.15)$$

Although $1/\mu$ may be identified with the radius of convergence of the mean size series unfortunately this does not always equal p_c . In particular, a Dlog Padé analysis of the $S(p)$ series for $d = 2$ and 3 (Sykes *et al* 1976a, d) shows that the radius of convergence is determined by a singularity on the negative real p -axis at $p = -p_0$. We have performed similar calculations for higher dimensions (see § 4) and conclude that as d increases p_0 moves further from the origin relative to p_c . It has not been possible to estimate p_0 with any precision, but very roughly

$$p_c/p_0 \approx 1.83, 1.65, 1.45, 1.25, 1.0 \quad (3.16)$$

for $d = 2, 3, 4, 5$ and 6 respectively. Such behaviour would tie in nicely with a critical dimension $d_c = 6$. But even if the estimates (3.16) are quite wrong, it seems likely that the singularity at p_c will eventually dominate the low density expansion of $S(p)$ for large enough d . This is what happens for the Bethe approximation (Fisher and Essam 1961)

$$S_B(p) = (1+p)/(1-\sigma p), \quad (p < p_c) \quad (3.17)$$

which has

$$p_c = 1/\sigma. \tag{3.18}$$

Hence for large enough d (or σ) we appear to have $\mu = 1/p_c$ and since the $(1/\sigma)$ -expansions are probably only asymptotic in any case, we take the exponential of (3.15) and write

$$1/p_c = \sigma(1 - \frac{1}{2}\sigma^{-1} - \frac{1}{2}\sigma^{-2} - 12\frac{7}{8}\sigma^{-3} - \dots). \tag{3.19}$$

Alternatively, we may invert this expression and obtain a $(1/\sigma)$ -expansion for p_c itself; namely

$$p_c = (1/\sigma)(1 + \frac{1}{2}\sigma^{-1} + 3\frac{3}{4}\sigma^{-2} + 20\frac{3}{4}\sigma^{-3} + \dots). \tag{3.20}$$

As expected the zeroth-order term is the result (3.18) of the Bethe approximation. The leading correction term is again of first order in $1/\sigma$; a similar result is suggested by the work of Domb (1972).

In contrast to (3.11), there are a sufficient number of terms in (3.20) to demonstrate explicitly that the smallest of them is attained, at least for $d = 2$ and 3. For $d = 3$ truncation after the smallest term yields an estimate which is too small by an amount equal to $\frac{2}{3}$ of the smallest term. We have therefore calculated approximations to p_c by truncating after the smallest term and adding $\frac{2}{3}$ of the smallest term *for all d* ; for $d = 4$ and 5 the smallest term is probably the last one, while for $d = 6$ it probably is not, although we have assumed it is for the purpose of these calculations. These estimates are denoted $p_c^{(\sigma)}$ in table 3. The accuracy for $d = 2$ is quite reasonable considering the expansion we are using is probably asymptotic. For $d = 3$, $p_c^{(\sigma)}$ coincides with the series estimate by construction and for $d = 4, 5$ and 6, $p_c^{(\sigma)}$ lies well within the numerical uncertainties of the series estimates.

We have also derived $1/\sigma$ -expansions for the mean number of clusters $K(p)$ and for the mean cluster size $S(p)$. These are the analogues of the $1/\sigma$ -expansions derived by Fisher and Gaunt for the free energy and zero field susceptibility of the Ising model (Fisher and Gaunt 1964, equations (5.3) and (5.19) respectively).

Starting with the mean number, first notice that the leading two terms of (2.2) constitute the mean number of clusters in the Bethe approximation for $p < p_c$

$$K_B(p) = p - \binom{d}{1}p^2. \tag{3.21}$$

Now from (3.1) each of the binomial coefficients $\binom{d}{s}$ in (2.2) can be replaced by a polynomial in σ of degree s , so that (2.2) can be written as

$$K(p) = K_B(p) + \sum_{r=4}^{\infty} p^r \sum_{t=0}^{[\frac{1}{2}r]} G_{r,t}^{\sigma} \sigma^t \tag{3.22}$$

where $[x]$ is the integer part of x , and the coefficients $G_{r,t}^{\sigma}$ can be calculated for all t for $r \leq 11$. In terms of the rescaled variable

$$x = \sigma p, \tag{3.23}$$

(3.22) becomes an expansion in powers of x in which the coefficient of x^r is a polynomial in inverse powers of σ of degree r , the lowest order term, however, being of degree $[\frac{1}{2}(r+1)]$. Regarding the series as a double series in x and $(1/\sigma)$ we may formally rearrange to obtain an expansion for the mean number of clusters in powers of $1/\sigma$.

Performing these manipulations we derive the result

$$\begin{aligned}
 K = K_B &+ \left(\frac{1}{8}x^4\right)\sigma^{-2} + \left(\frac{1}{12}x^6\right)\sigma^{-3} + \left(-\frac{1}{8}x^4 - \frac{1}{4}x^6 - \frac{1}{6}x^7 + \frac{7}{16}x^8\right)\sigma^{-4} \\
 &+ \left(-\frac{1}{12}x^6 + \frac{1}{2}x^7 - 2\frac{1}{16}x^8 - \frac{7}{8}x^9 + 3\frac{3}{20}x^{10}\right)\sigma^{-5} \\
 &+ \left(\frac{1}{4}x^6 + \frac{1}{6}x^7 + 4\frac{9}{16}x^8 + 13\frac{1}{2}x^9 - 35\frac{5}{12}x^{10} + \dots\right)\sigma^{-6} \\
 &+ \left(-\frac{1}{2}x^7 + 2\frac{15}{16}x^8 - 21\frac{7}{8}x^9 + 132\frac{11}{24}x^{10} + \dots\right)\sigma^{-7} \\
 &+ \left(-5x^8 - 13\frac{1}{2}x^9 - 137\frac{11}{24}x^{10} + \dots\right)\sigma^{-8} \\
 &+ \left(23\frac{3}{4}x^9 - 135\frac{73}{120}x^{10} + \dots\right)\sigma^{-9} \\
 &+ \left(172\frac{7}{8}x^{10} + \dots\right)\sigma^{-10} + \dots
 \end{aligned} \tag{3.24}$$

which is correct to order x^{10} and to order $(1/\sigma)^5$.

The first term on the right-hand side of (3.24), corresponding to $(1/\sigma) \rightarrow 0$, is just the Bethe approximation for $p < p_c$ ($x < 1$). In as far as the truncated series in $1/\sigma$ is a good representation of $K(p)$ one is justified in concluding that the Bethe approximation becomes more accurate as $\sigma \rightarrow \infty$. Notice that the leading correction term is now of order $(1/\sigma)^2$ rather than of order $(1/\sigma)$. The corresponding expansion for the free energy $f = -F/kT = \ln Z$ of the Ising model is (Fisher and Gaunt 1964, equation (5.3))

$$f = f_B + \left(\frac{1}{8}x^4\right)\sigma^{-2} + \left(\frac{1}{3}x^6\right)\sigma^{-3} + \left(-\frac{1}{8}x^4 - \frac{3}{4}x^6 + 1\frac{11}{16}x^8\right)\sigma^{-4} + \dots \tag{3.25}$$

where f_B is just the Bethe approximation for $T > T_c$. The expansions (3.24) and (3.25) are rather similar in form; indeed the leading correction terms which are both of order $(1/\sigma)^2$ are identical while the second-order corrections are only slightly different. Of course, the higher-order corrections differ more and more. This similarity in form reflects the close formal analogy which exists between the Ising ferromagnet and the percolation problem (Kasteleyn and Fortuin 1969).

If one sets $1/\sigma = 1$ in (3.24) one discovers that the coefficient of each power of x vanishes identically. This simply corresponds to the fact that the Bethe approximation is exact for the one-dimensional linear chain ($\sigma = 1, \nu = 2, d = 1$).

Evidently the coefficient of $(1/\sigma)^m$ is a polynomial in x , the term of lowest degree being x^m and that of highest degree being x^{2m} . Although each coefficient is merely a finite polynomial in x and hence is a non-singular function of p , it is clear that the series in $(1/\sigma)$ can only represent the mean number $K(p)$ for $p < p_c$ i.e. only for $x < x_c = x_c(\sigma)$. This strongly suggests that the series in $(1/\sigma)$ for fixed x is divergent if x is large enough.

One may also expand the mean cluster size $S(p)$ in powers of $1/\sigma$. This is most easily done, at least in principle, by starting with the expression (3.12) for the expansion coefficients b_r , multiplying by p^r and summing from $r = 6$ to ∞ . After some rather heavy algebraic manipulation we find

$$\begin{aligned}
 S = S_B &+ \frac{x^3}{(1-x)^2} \left(-1\frac{1}{2}\right)\sigma^{-1} + \frac{x^3}{(1-x)^3} \left(2x - 2\frac{1}{2}x^2 + 2\frac{3}{4}x^3\right)\sigma^{-2} \\
 &+ \frac{x^3}{(1-x)^4} \left(1\frac{1}{2} - 3x + 4\frac{1}{2}x^2 - 35\frac{3}{4}x^4 + 52\frac{3}{4}x^5 - 23\frac{3}{8}x^6\right)\sigma^{-3} + \dots
 \end{aligned} \tag{3.26}$$

where the leading term, S_B , is the Bethe approximation for $p < p_c$ given by (3.17).

Alternatively, and perhaps more interestingly, one may define the recurrence relation

$$b_r = 2\sigma b_{r-1} - \sigma^2 b_{r-2} + d_r, \quad (r = 3, 4, 5, \dots) \tag{3.27}$$

where $b_1 = \sigma + 1$ and $b_2 = \sigma(\sigma + 1)$. If all the correction coefficients $d_r \equiv 0$, then (3.27) generates the low density coefficients of the Bethe approximation. Similar recurrence relations exist for the coefficients of the high temperature susceptibility and generating function for self-avoiding walks; in these cases the correction coefficients have direct graph-theoretical interpretations (Sykes 1961). By solving the recurrence relation generally the series coefficients b_r are given explicitly in terms of the d_r by

$$b_r(d) = q\sigma^{r-1} + \sum_{k=3}^r d_k(r+1-k)\sigma^{r-k}. \tag{3.28}$$

Multiplication by p^r followed by summation from $r = 1$ to ∞ yields

$$S(p) = \frac{1+p}{1-\sigma p} + \sum_{r=1}^{\infty} \sum_{k=3}^r d_k(r+1-k)p^r\sigma^{r-k} \tag{3.29}$$

where the first term is the Bethe approximation (3.17). On writing $p = x/\sigma$, interchanging the order of summation and summing on $j = r - k$, we get

$$S = S_B + \sum_{k=3}^{\infty} (d_k/\sigma^k) \frac{x^k}{(1-x)^2}. \tag{3.30}$$

Expressing d_3, d_4, \dots, d_8 as polynomials in σ by using (3.27), (2.6) and (3.1), we find

$$\begin{aligned} d_3 &= -\frac{1}{2}\sigma^2 + 1\frac{1}{2} \\ d_4 &= 2\sigma^2 - 2 \\ d_5 &= -\frac{1}{2}\sigma^3 + 3\sigma^2 + \frac{1}{2}\sigma - 3 \\ d_6 &= 2\frac{1}{4}\sigma^4 + 6\sigma^3 - 35\sigma^2 - 6\sigma + 32\frac{3}{4} \\ d_7 &= 2\frac{1}{4}\sigma^5 - 26\frac{3}{4}\sigma^4 + 111\frac{1}{6}\sigma^3 - 128\frac{1}{2}\sigma^2 - 153\frac{5}{12}\sigma + 115\frac{1}{4} \\ d_8 &= 2\frac{1}{4}\sigma^6 - 6\frac{3}{4}\sigma^5 + 173\frac{1}{4}\sigma^4 - 1284\frac{2}{3}\sigma^3 + 2167\frac{3}{4}\sigma^2 + 1291\frac{5}{12}\sigma - 2343\frac{1}{4} \end{aligned} \tag{3.31}$$

where for $k \geq 4$, d_k is a polynomial of degree $(k - 2)$. Substituting (3.31) into (3.30), collecting up terms in $1/\sigma$ and performing the infinite sums for the terms in $(1/\sigma)^2$ and $(1/\sigma)^3$, which yield extra factors $(1-x)^{-1}$ and $(1-x)^{-2}$ respectively, we finally obtain (3.26).

The Bethe approximation (3.17) has a simple pole at $x = 1$. The coefficient of $(1/\sigma)^m$ in (3.26) appears to have the form

$$x^3(k_0 + k_1x + k_2x^2 + \dots + k_{3(m-1)}x^{3(m-1)})(1-x)^{-(m+1)}, \tag{3.32}$$

and hence diverges increasingly strongly at $x = 1$ as m increases. Of course the divergence of the $(1/\sigma)$ -expansion to all orders at $x = 1$ is an artifact and does not imply that $S(x/\sigma)$ has any singularity at $x = 1$. Notice that in contrast to the mean number expansion (3.24) the leading correction term in (3.26) is now of first order in $(1/\sigma)$. This means that the Ising/percolation analogy mentioned earlier is not now as close, since the analogous expansion for the reduced susceptibility of the Ising model (Fisher and

Gaunt 1964, equation (5.19))

$$\chi = \chi_B - \frac{x^4}{(1-x)^2} \sigma^{-2} + O(\sigma^{-3}), \quad (3.33)$$

where χ_B is the Bethe approximation for $T > T_c$, has its first correction term of second order.

4. Series analysis

In this section we analyse the low density expansion of the mean size of clusters $S(p)$, and the expansion of the generating function $A(z)$ for the total number of clusters with s -sites, N_s , namely

$$A(z) = 1 + \sum_{s=1}^{\infty} N_s z^s. \quad (4.1)$$

Our aim is to examine the question of a critical dimension; for percolation processes, Toulouse (1974) has suggested this must be $d_c = 6$.

The analysis of the mean size series $S(p)$ is complicated by the presence of the non-physical singularity on the real negative p -axis at $p = -p_0$. As mentioned in the last section, it is this singularity which ultimately dominates the behaviour of the series coefficients for small d . However, the *early* coefficients are dominated by the strong physical singularity at p_c ; the only effect on the initial coefficients of the much weaker singularity at $-p_0$ is to cause a characteristic odd/even oscillation in the ratios μ_n of successive coefficients. Hence an analysis of the physical singularity may be attempted using the basic ratio method (Gaunt and Guttmann 1974). In practice, the non-physical singularity proves to be rather troublesome and consequently our results are not very precise. For this reason we merely outline the procedure that we have followed suppressing most of the details.

Because of the odd/even oscillations, we first calculate the quantities $\mu_n^* = \frac{1}{2}[n\mu_n - (n-2)\mu_{n-2}]$, which are the intercepts obtained by extrapolating linearly against $1/n$ alternate pairs of ratios. Taking successive averages $\frac{1}{2}(\mu_n^* + \mu_{n-1}^*)$ smooths out the oscillations and extrapolating to $n = \infty$ yields reasonably good estimates of the limit $\mu = 1/p_c$. Corresponding estimates of γ may be obtained by first calculating $\gamma_n = 1 + n(\mu_n - \mu)/\mu$ followed by extrapolation of the smoother averages $\frac{1}{2}(\gamma_n + \gamma_{n-1})$.

We have also studied the Dlog Padé approximants to $S(p)$. The last few entries in each of the main diagonal and off-diagonal sequences were used to estimate p_c . The corresponding value of γ was then read from a pole-residue plot. The location of the closest singularity on the negative p -axis was also studied and rough estimates were given in (3.16).

Our best overall estimates of p_c and γ for $d = 4, 5$ and 6 are presented in table 3. For completeness the corresponding values for $d = 2$ and 3 are also tabulated (Sykes *et al* 1976a, d). Roughly speaking, as d increases, the configurational data 'samples' the lattice less and less representatively, and the uncertainties in both p_c and γ increase accordingly. Table 3 confirms that to within numerical accuracy the exponent γ attains the mean field value $\gamma = 1$ in six dimensions, that is $d_c = 6$. In figure 1 values of γ for $d = 2$ to 6 are plotted against d and are seen to vary reasonably smoothly. The broken line is the prediction of Harris *et al* (1975) who used a renormalization-group approach. To first order in $\epsilon = 6 - d$, they found

$$\gamma = 1 + \frac{1}{7}\epsilon. \quad (4.2)$$

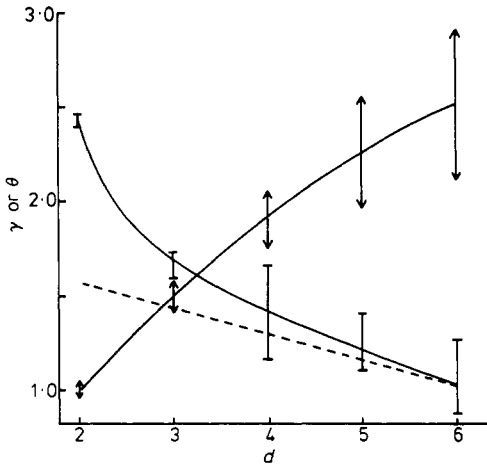


Figure 1. Exponents γ and θ plotted as functions of dimension d . The broken curve shows the result of the renormalization group expansion to first order in ϵ .

Although the ϵ -expansion result gives the correct qualitative trend for small ϵ , it is not in quantitative agreement, lying below the true curve.

We turn now to the expansion (4.1) of the generating function $A(z)$. According to (1.2), $A(z)$ should exhibit a singularity on the real positive z -axis of the form (Gaunt and Guttmann 1974)

$$A(z) \approx A_0 - A_1(1 - \lambda z)^{\theta - 1}, \quad (\theta > 1, z \rightarrow 1/\lambda -) \tag{4.3}$$

where $\theta = 1$ is interpreted as a logarithmic divergence. Since the N_s are necessarily positive, the singularity at $z = z_c = 1/\lambda$ must lie on the circle of convergence; there can be no closer singularity on the negative z -axis, for example. This is confirmed by the Dlog Padé approximants, according to which the first singularity on the negative axis is more than $2z_c$ from $z = 0$ for any d . (In addition, there is no evidence of any singularities in the complex z -plane). In this respect the analysis of the $A(z)$ series is simpler than the $S(p)$ series. Unfortunately, it appears that there is a confluent singularity at $z = z_c$ and this slows down the convergence considerably. For this reason we again confine ourselves to outlining our procedure but omitting all details.

We begin by estimating the exponent θ from the sequence

$$\theta_s = s \left(1 - \frac{\lambda_s}{\lambda'} \right) \quad (s = 1, 2, 3, \dots)$$

where $\lambda_s = N_s/N_{s-1}$ is the ratio of successive coefficients and λ' is an estimate of the limit λ . As the ratios λ_s are so smooth we have used as the s th estimate for λ' , the quantity $s\lambda_s - (s-1)\lambda_{s-1}$ which is the intercept obtained by extrapolating linearly against $1/s$ adjacent pairs of ratios. For s sufficiently large, the θ_s form a slowly increasing sequence (because of the confluent singularity) which is not easily extrapolated. Plotting against $1/s$ produces curves with quite a lot of curvature which we have tried to allow for using N -shifts and other devices (Gaunt and Guttmann 1974). Our best estimates of θ obtained in this way are presented in table 3 for $d = 2$ to 6.

Adopting the central values of θ we now estimate the corresponding growth parameter λ . Both the linear intercepts, $s\lambda_s - (s-1)\lambda_{s-1}$, just defined and the quantities $s\lambda_s/(s-\theta)$, provide sequences of estimates for λ which for sufficiently large s are monotonically increasing and decreasing, respectively. From these we obtain the

estimates given in table 3; the uncertainty in θ would yield an additional uncertainty in λ of the same order of magnitude as that quoted. The central value of θ and the best estimate of λ have been given previously for $d = 2$ and 3 (Sykes and Glen 1976, Sykes *et al* 1976d).

The above estimates of θ and λ are broadly confirmed by a Padé approximant analysis, but with larger uncertainties. The only point worth mentioning here is that the analysis must not be performed on $A(z)$ but on the expansion of the derivative function dA/dz or d^2A/dz^2 , chosen so that the asymptotic form (4.3) is converted into an algebraic divergence.

The values of θ for $d = 2$ to 6 are plotted in figure 1 and seem to vary smoothly with d . This figure and table 3 suggest strongly that the exponent θ also reaches its mean-field value $\theta = 2\frac{1}{2}$ in six dimensions. In other words, it seems reasonable to conjecture that here too $d_c = 6$.

5. Conclusions

The data available is difficult to extrapolate with precision. Our final estimates for p_c and γ in table 3 are in very reasonable agreement with the Monte Carlo estimates, $p_c^{(MC)}$ and $\gamma^{(MC)}(d)$, of Kirkpatrick (1976). Within the accuracy attainable they support the hypothesis of Toulouse (1974) that $d_c = 6$ for the percolation problem. For the closely related cluster growth problem we have been led to make the hypothesis that $d_c = 6$ in this case also.

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