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Series study of random percolation in three dimensions

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Abstract. New high-density series data for the mean number, percolation probability and 'susceptibility' of finite clusters are presented for bond and site percolation on four standard three-dimensional lattices. Our Padé approximant analysis of both high- and low-density series makes particular use of the rather precise unbiased estimates of the percolation threshold, p_c , obtained recently by Heermann and Stauffer for the simple cubic lattice. For this lattice we obtain the biased estimate $\gamma = 1.73 \pm 0.03$ for the site problem and a similar estimate but with larger uncertainties for the bond problem. Such a value is significantly larger than earlier series estimates. Assuming γ to be universal we obtain precise, although biased, estimates of p_c for both bond and site percolation on all four lattices. Using the bond estimates of p_c we find an overall biased estimate of $\beta = 0.454 \pm 0.008$ for bond percolation on *all* three-dimensional lattices. (The corresponding site problem requires further study.) Scaling estimates of other critical exponents are $\alpha = -0.64 \pm 0.05$, $\delta = 4.81 \pm 0.14$, $\Delta = 2.18 \pm 0.04$, $\nu = 0.88 \pm 0.02$ and $\eta = 0.03 \pm 0.03$.

1. Introduction

At the present time, none of the critical exponents for the percolation problem (Stauffer 1979, Essam 1980) are known exactly for any of the two- or three-dimensional lattices. However, in two dimensions, the well known relationship (Kasteleyn and Fortuin 1969, Giri *et al* 1977, Kunz and Wu 1978) between percolation and the Potts model (Wu 1982) has led to conjectures (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980) for the percolation exponents that are strongly supported by numerical estimates obtained from series expansions (Domb and Pearce 1976, Sykes *et al* 1976c, Blease *et al* 1978, Dunn *et al* 1975, Essam *et al* 1976, Adler and Privman 1981, Adler *et al* 1982, Gaunt and Sykes 1976) and other techniques (Leath and Reich 1978, Eschbach *et al* 1981, Blöte *et al* 1981). In three dimensions, the situation is less satisfactory and there is no general consensus concerning the values of the critical exponents obtained from series expansions, Monte Carlo (MC) simulations or any other technique. The exponent β describing the behaviour of the percolation probability close to the critical percolation threshold p_c is a typical example. Sykes *et al* (1976a) have given a series estimate for site percolation on the face-centred cubic (FCC) lattice of

$$\beta = 0.42 \pm 0.06 \quad \text{FCC(S)}. \quad (1.1)$$

A more precise (but not necessarily more accurate) series estimate was obtained by Blease *et al* (1976) for bond percolation on the FCC lattice,

$$\beta = 0.47 \pm 0.02 \quad \text{FCC(B)}. \quad (1.2)$$

On the other hand, a typical MC estimate of β , this time for the simple cubic (sc) site problem, is (Kirkpatrick 1976)

$$\beta = 0.39 \pm 0.02 \quad \text{sc(s)}. \quad (1.3)$$

Other MC estimates include $\beta = 0.41 \pm 0.01$ (Sur *et al* 1976) and $\beta = 0.42 \pm 0.02$ (Nakanishi and Stanley 1980). Thus, we see that either the uncertainties (or more precisely the confidence limits) are quite large as in (1.1) or else, as in (1.2) and (1.3), the uncertainties are smaller but the estimates are mutually inconsistent. Similar difficulties beset the estimation of other percolation exponents in three dimensions.

Quite recently, renewed efforts have been made to obtain more accurate estimates of percolation exponents in three dimensions. Gaunt *et al* (1981) have utilised three different definitions of the percolation probability for the simple cubic bond problem all of which can be shown rigorously to have the same critical exponent β . By deriving and analysing long series expansions for all three of these functions they found

$$\beta = 0.463 \pm 0.013 - 12\Delta p_c \quad \text{sc(B)} \quad (1.4)$$

where $\Delta p_c = p_c - 0.247$. The first (inherent) uncertainty reflects the consistency of the numerical analysis while the second term describes the effect of uncertainties in the location of p_c . (In contrast to two dimensions, p_c is not known exactly for either site or bond percolation on any three-dimensional lattice.) As emphasised by Gaunt *et al*, the lack of agreed, precise and unbiased estimates of p_c in three dimensions is a serious obstacle to the determination of precise estimates of critical exponents by series methods. For the simple cubic lattice, this deficiency has been remedied by the MC simulations of Heermann and Stauffer (1981, to be referred to as HS). Using system sizes up to 100^3 sites and finite-size scaling theory, they obtained a precise and unbiased estimate in the case of site percolation of

$$p_c = 0.3117 \pm 0.0003 \quad \text{sc(s)}. \quad (1.5)$$

For the corresponding bond problem, a smaller investment of effort resulted in the rather less precise estimate of

$$p_c = 0.248 \pm 0.001 \quad \text{sc(B)}. \quad (1.6)$$

In the present paper we continue our earlier study by presenting some new high-density series data and performing a preliminary analysis in which the estimates (1.6) and especially (1.5) play a central role. We obtain new, precise, biased estimates of p_c for site and bond percolation on all three-dimensional lattices and study the critical exponents γ , β , γ' and δ , making new, biased and reasonably precise estimates of γ and β . Although precise estimates of critical amplitudes are also highly desirable for calculating universal critical amplitude ratios (Aharony 1980), we believe that further efforts in this direction are, for the moment, premature.

We have derived high-density series in powers of $q (= 1-p)$, the density of unoccupied sites, for the face-centred cubic (FCC), body-centred cubic (BCC), simple cubic (sc) and diamond (D) lattices. The expansions are for the mean number K of finite clusters per lattice site, the percolation probability P and the 'susceptibility' χ per lattice site which is closely related to the mean size S of finite clusters. (For the definitions, see Sykes *et al* (1976b) and equation (2.19).) They are given in the appendices up to order q^N , where for the bond problem $N = 62(\text{FCC}), 47(\text{BCC}), 36(\text{sc}), 25(\text{D})$ and for the site problem $N = 47(\text{FCC}), 39(\text{BCC}), 33(\text{sc}), 20(\text{D})$. Further details and additional data will be published in due course. Prior to this paper, the only

published data of this kind were for the percolation probability up to q^{33} for the sc bond problem (Gaunt *et al* 1981) and up to q^{45} for the FCC site problem—although in the latter case the last four coefficients given by Sykes *et al* (1976a) are now known to contain small errors. As already mentioned, expansions based upon slightly different definitions of the percolation probability for bond percolation have been given for the sc lattice up to q^{30} by Gaunt *et al* (1981) and for the FCC lattice up to q^{67} by Blease *et al* (1976), whose papers should be consulted for details of the alternative definitions.

In this preliminary communication, we have based our series analysis on the assumption of simple power-law singularities. We neglect confluent singular terms despite the knowledge that they appear to be responsible for some well known universality-violating puzzles, e.g. in the three-dimensional Ising model (Nickel 1982, Zinn-Justin 1981, Roskies 1981) and in the two-dimensional percolation problem (Adler *et al* 1982). In these cases, however, the discrepancy was only about 1% and 1.7%, respectively, in contrast to the present situation where the discrepancy between (1.2) and (1.3), say, is almost 20%. In the first instance, therefore, we are interested in discovering to what extent, if any, such a discrepancy can be resolved using conventional techniques coupled with much more extensive series data. In any case, such numerical evidence as there is (J Adler, private communication) suggests that for percolation in three dimensions the leading confluent exponent Δ_1 is close to 1 and does not seem to modify the dominant exponent as much as in the two cases mentioned above. A renormalisation group (RG) field-theoretic calculation by Houghton *et al* (1978) based upon resummation of the ε expansion gives a correction-to-scaling exponent ω (Wegner 1972) in the range 0.914–1.13, while Reeve *et al* (1982) using the methods of Baker *et al* (1976) give $\omega \approx 1.5$. The exponent ω , which is calculated from the derivative of the β function evaluated at the fixed point, is related to Δ_1 through $\Delta_1 = \omega\nu$ where ν is the critical exponent for the correlation length and appears to lie in the range 0.8–0.9 (Essam 1980, Stauffer 1979).

While paying particular attention to the analysis of the new high-density series, we have also taken the opportunity to re-analyse the corresponding low-density series (Sykes *et al* 1976d). Our main tool has been pole-residue plots derived from Dlog Padé approximants (Gaunt and Guttmann 1974). For the high-density series, many of the initial coefficients are zero and, consequently, we have found it useful to consider Dlog Padé approximants from a wide region of the Padé table (and not just the central and main off-diagonal sequences). For many of the series, including the low-density ones, the Dlog Padé approximants detect non-physical singularities (and, for the high-density series, in relatively large numbers) lying closer to the origin than p_c either on the negative real axis or in the complex plane. These singularities frustrate any attempt at a 'clean' ratio analysis (Gaunt and Guttmann 1974), even of the low-density series, and interference from them will undoubtedly slow down convergence of the Dlog Padé approximants close to p_c . At high densities, the non-physical singularities cause least disturbance to the percolation probability series, more to the susceptibility and most to the mean number series. (No further reference will be made to the mean number series since our analysis fails at both high and low densities.) The above pattern of behaviour parallels that observed for the low-temperature series of the three-dimensional Ising model (see Gaunt and Guttmann 1974, § III.D) with the spontaneous magnetisation replacing the percolation probability, the initial susceptibility replacing the susceptibility or mean size and the zero-field free energy replacing the mean number (Kasteleyn and Fortuin 1969).

This paper is divided into three sections and two appendices. In the next section, we present our analysis of the low- and high-density series for the standard three-dimensional lattices and give new biased estimates of the critical exponents γ and β , and of p_c for both bond and site percolation. In § 3, we summarise our main results, making scaling predictions for the remaining critical exponents, and compare our results with those obtained by other workers. The new high-density series data are collected together in the appendices.

2. Series analysis

2.1. Low-density mean size

We begin by re-analysing the low-density mean size series, $S(p)$, for the site problem on the sc lattice. We have chosen this particular series, to be found in the paper by Sykes *et al* (1976d), because of the existence of a precise unbiased estimate, (1.5), of p_c due to HS. Although all the series coefficients presently available are positive, a ratio analysis (Gaunt and Guttmann 1974) is unsatisfactory since the ratios of coefficients are influenced and ultimately dominated by a non-physical singularity on the negative real p axis lying closer to the origin than does p_c . Instead we have formed Dlog Padé approximants (Gaunt and Guttmann 1974) to $S(p)$ and plotted in figure 1 the location of the appropriate pole against the corresponding residue. From these results, which define a relatively smooth curve (pole-residue plot) we may read off a biased estimate of the critical exponent γ corresponding to (1.5), namely

$$\gamma = 1.73 \pm 0.02 + 33\Delta p_c \quad \text{sc(s)} \quad (2.1)$$

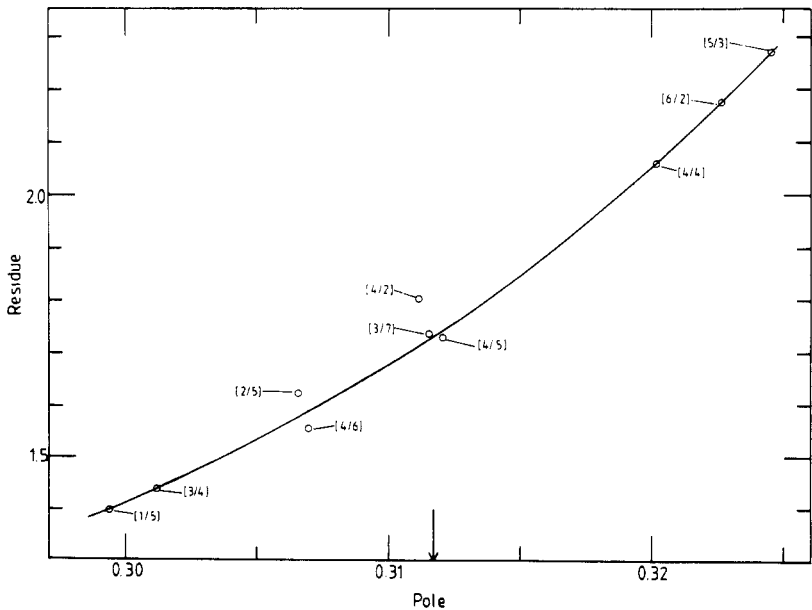


Figure 1. Pole-residue plot. Low-density expansion of mean size $S(p)$, sc site problem. The arrow locates p_c as given by HS (see equation (1.5)).

where $\Delta p_c = p_c - 0.3117$. Assuming that $|\Delta p_c| \leq 0.0003$ as in (1.5) gives

$$\gamma = 1.73 \pm 0.03 \quad \text{SC(S)}. \quad (2.2)$$

HS also gave an unbiased estimate, (1.6), of p_c for the bond problem on the SC lattice. From the pole-residue plot obtained using the Dlog Padé approximants to the $S(p)$ series (Sykes *et al* 1976d) we find, corresponding to (1.6),

$$\gamma = 1.74 \pm 0.03 + 73\Delta p_c \quad \text{SC(B)} \quad (2.3)$$

where $\Delta p_c = p_c - 0.248$. If $|\Delta p_c| \leq 0.001$ as in (1.6), this gives

$$\gamma = 1.74 \pm 0.10 \quad \text{SC(B)}. \quad (2.4)$$

The fact that the uncertainty in (2.4) is so much larger than that in (2.2) reflects, to a large extent, the correspondingly large uncertainties in p_c (cf (1.5) and (1.6)). (Note that the *inherent* uncertainties in (2.1) and (2.3) are comparable.) However, the central estimates in (2.2) and (2.4) are quite close and support the hypothesis of a common value of γ for both bond and site percolation on the SC lattice. According to the universality hypothesis (Essam 1980, Stauffer 1979), γ should be the same for both bond and site percolation on *all* three-dimensional lattices. Hence, assuming a universal value of γ , we adopt (2.2) as our best (biased) estimate.

We now use (2.2) in conjunction with pole-residue plots from Dlog Padé approximants to $S(p)$ series (Sykes *et al* 1976d) to obtain precise but biased estimates of p_c for both bond and site problems on all the standard three-dimensional lattices. Thus, we find

$$\begin{aligned} p_c &= 0.1198 \pm 0.0003 && \text{FCC(B)} \\ &= 0.1795 \pm 0.0003 && \text{BCC(B)} \\ &= 0.2479 \pm 0.0004 && \text{SC(B)} \\ &= 0.3886 \pm 0.0005 && \text{D(B)} \end{aligned} \quad (2.5)$$

and

$$\begin{aligned} p_c &= 0.1998 \pm 0.0006 && \text{FCC(S)} \\ &= 0.2464 \pm 0.0007 && \text{BCC(S)} \\ &= 0.3117 \pm 0.0003 && \text{SC(S)} \\ &= 0.4299 \bullet 0.0008 && \text{D(S)} \end{aligned} \quad (2.6)$$

where for the SC site problem we repeat the estimate in (1.5). For the SC bond problem, the estimate in (2.5) differs from (1.6) because of the difference in (2.2) and (2.4).

We have obtained new estimates of p_c and of γ by re-analysing our old series (Sykes *et al* 1976d) for $S(p)$; that is, using no additional coefficients. The increased precision has resulted solely from the use of the more precise estimate, (1.5), of p_c for the SC site problem. Our new estimates of p_c in (2.5) and (2.6) are larger than earlier estimates (Sykes *et al* 1976d, Dunn *et al* 1975) in all cases, although with one exception the new estimates lie well within the relatively large uncertainties of the earlier estimates. The exception is the FCC bond problem for which the earlier estimate of p_c was the most precise (Dunn *et al* 1975); however, the uncertainties in the new and earlier estimates of p_c just overlap even in this case. Our new estimate (2.2) of

γ is significantly larger than the central value in our earlier estimate (Sykes *et al* 1976d),

$$\gamma = 1.66 \pm 0.07, \quad (2.7)$$

although the large uncertainties in (2.7) just include the central value in (2.2). This increase in the magnitude of our central estimate of γ is due to the increases mentioned above in our estimates of p_c . To demonstrate this, we note that (2.7) was derived from a pole-residue plot for the FCC bond problem which gave the result (Sykes *et al* 1976d, equation (3.3))

$$\gamma = 1.66 \pm 0.02 + 90\Delta p_c \quad \text{FCC(B)} \quad (2.8)$$

where $\Delta p_c = p_c - 0.1190$. Assuming that $|\Delta p_c| \leq 0.0005$ (Dunn *et al* 1975) gives (2.7). However, if we use our new central estimate of $p_c = 0.1198$, then (2.8) gives a central value of $\gamma = 1.732$ in excellent agreement with the central estimate in (2.2).

2.2. Percolation probability

In contrast to low densities, many of the high-density series have been extended by a significant number of terms. We now use the more precise estimates of p_c , just determined, to analyse these expansions and determine biased estimates of critical exponents. The best converged series at high densities are those for the percolation probability. For the SC bond problem the recent work of Gaunt *et al* (1981) gave (1.4), which in conjunction with our new estimate, (2.5), of p_c gives

$$\beta = 0.452 \pm 0.018 \quad \text{SC(B)}. \quad (2.9)$$

The three extra coefficients given in appendix 1 do not change (1.4) and hence (2.9) is unaffected also. For the FCC bond problem, we have used the analogous work of Blease *et al* (1976) who give

$$\beta = 0.474 \pm 0.002 - 24\Delta p_c \quad \text{FCC(B)} \quad (2.10)$$

where $\Delta p_c = p_c - 0.1190$. Use of (2.5) for p_c then yields

$$\beta = 0.455 \pm 0.009 \quad \text{FCC(B)}. \quad (2.11)$$

Similarly, we have constructed the pole-residue plots shown in figures 2 and 3 for the D and BCC bond problems, respectively, using the series for $P(q)$ given in appendix 1. We find

$$\beta = 0.447 \pm 0.009 - 11\Delta p_c \quad \text{D(B)} \quad (2.12)$$

where $\Delta p_c = p_c - 0.3886$, and

$$\beta = 0.456 \pm 0.020 - 18\Delta p_c \quad \text{BCC(B)} \quad (2.13)$$

where $\Delta p_c = p_c - 0.1795$. Assuming the uncertainties given in (2.5) then gives

$$\beta = 0.447 \pm 0.015 \quad \text{D(B)} \quad (2.14)$$

and

$$\beta = 0.456 \pm 0.025 \quad \text{BCC(B)}. \quad (2.15)$$

The estimates in (2.9), (2.11), (2.14) and (2.15) provide strong support for a universal value of β for all three-dimensional bond problems. To our knowledge this is the first time that reasonably precise estimates of β have been given for all four

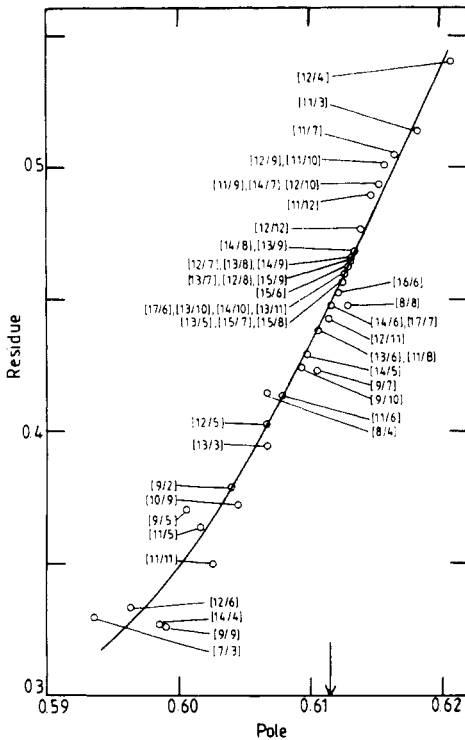


Figure 2. Pole-residue plot. High-density expansion of percolation probability $P(q)$, D bond problem. The arrow locates p_c as given in (2.5).

standard lattices which actually agree to within their estimated uncertainties. By considering the overlap range of the four estimates, and assuming a common value, we obtain an overall bond estimate for $d = 3$ dimensions of

$$\beta = 0.454 \pm 0.008 \quad d = 3 \text{ (B)}. \tag{2.16}$$

All the allowed values of β for all four lattices satisfy

$$0.431 \leq \beta \leq 0.481 \quad d = 3 \text{ (B)}. \tag{2.17}$$

We turn now to the $P(q)$ series for the *site* problem, where the corresponding analysis turns out to be much less satisfactory. Forming pole-residue plots as before yields the estimates

$$\begin{aligned} \beta &= 0.405 \pm 0.025 && \text{FCC(S)} \\ &= 0.377 \pm 0.012 && \text{BCC(S)} \\ &= 0.403 \pm 0.008 && \text{SC(S)} \\ &= 0.365 \pm 0.08 && \text{D(S)} \end{aligned} \tag{2.18}$$

where the uncertainties include an inherent uncertainty plus a contribution arising from the uncertainties in p_c given in (2.6). There is now *no* region where the estimates overlap for all four lattices and the two most precise estimates (namely, those for the BCC and SC lattices) share no overlap region. If we reject the unlikely notion of a

significant that of all the central site estimates of β in (2.18) it is that for the FCC lattice which is closest to our best bond estimate (2.16). Furthermore, the maximum value of β permitted by the quoted uncertainties for the FCC site problem falls only just short of the allowed range (2.17) for the bond problem.

2.3. Exponents γ' and δ

We conclude this section by summarising our results for a number of series, re-analysis of which has not substantially changed earlier conclusions. To study the exponent γ' we have, following Sykes *et al* (1976c), analysed high-density expansions for the susceptibility, $\chi(q)$, and also for the mean size $S(q)$, given by

$$S(q) = \chi(q)/p_t \quad (2.19)$$

where $p_t = p(1 - P(q))$ is the density of occupied sites belonging to finite clusters. Although χ and S must have the same dominant singularity with exponent γ' , the exponent associated with the leading confluent term may or may not be the same for the two functions. Despite much longer series than previously available, our Padé approximant analysis, based upon pole-residue plots, is inconclusive although not inconsistent with the scaling result $\gamma' = \gamma$. However, two rather general features may be discerned. First, it appears that the series for the bond problem converge more rapidly than for the site problem and, second, that $\chi(q)$ converges more rapidly than $S(q)$, probably in all cases. This second feature has also been commented upon by other workers (Hoshen *et al* 1979, Nakanishi and Stanley 1980). Thus, for the most favourable series, namely $\chi(q)$ for the bond problem, the *apparent value* of γ' lies between 1.57 and 1.69 for all four lattices—a little smaller than the probable value of $\gamma' = \gamma \approx 1.73$. On the other hand, the bond series for $S(q)$ give an apparent exponent lying between 1.14 and 1.24 for all four lattices. Such a large difference between $\chi(q)$ and $S(q)$ may indicate that the confluent correction terms for these two functions are associated with different exponents. By far the best results for the site problem are obtained with the $\chi(q)$ series for the FCC lattice which gives an apparent value of $\gamma' \approx 1.84$, a little larger than the scaling value of $\gamma' = \gamma \approx 1.73$.

Finally, our more precise estimates, (2.5) and (2.6), of p_c have caused us to re-examine the series analysis by Gaunt (1977) of the exponent δ . Gaunt made the overall estimate of

$$\delta = 5.0 \pm 0.8 \quad (2.20)$$

plus an additional uncertainty of about ± 0.5 due to uncertainties in p_c . More specifically, it turns out that an *increase* in the value of p_c from the central values given by Sykes *et al* (1976d) has the effect of *increasing* the estimates of δ also, i.e. a *lowering* of the plots given in figure 1 of Gaunt (1977). In fact, our new estimates of p_c are larger than the earlier estimates in all cases and by an amount which increases the estimates of δ by about half the maximum allowed by Gaunt (1977), i.e. by about 0.25. Such values of δ would be more in line with the estimate of $\delta \approx 5.3$ quoted, without uncertainties, by Nakanishi and Stanley (1980) than with the central value in (2.20). Unfortunately, a change of this magnitude is largely swamped by the much greater inherent uncertainties in δ of ± 0.8 . Further analysis aimed at reducing the size of these inherent uncertainties is being undertaken.

3. Summary and conclusions

We have derived extensive new high-density series data for bond and site percolation on the standard three-dimensional lattices. These series and existing low-density series have been analysed by Padé approximant techniques involving pole-residue plots. The analysis relies heavily on a rather precise unbiased estimate of p_c obtained recently by Heermann and Stauffer (1981) for the site problem on the sc lattice. Our results include precise although biased estimates of p_c for all other site and bond problems (see (2.5) and (2.6)). Apart from the work of HS, most other work aimed at providing precise estimates of p_c seems to have been confined to the honeycomb and square site problems in two dimensions (Vicsek and Kertész 1981, Derrida and de Seze 1982, Djordjevic *et al* 1982). We hope that our present estimates of p_c will provide some stimulus for further work on three-dimensional site and bond problems and that precise unbiased estimates of p_c will soon be forthcoming.

In addition to estimating p_c , we have obtained reasonably precise biased estimates of the universal critical exponents γ and β , namely

$$\gamma = 1.73 \pm 0.03 \quad (3.1)$$

$$\beta = 0.454 \pm 0.008. \quad (3.2)$$

The value (3.1) of γ is obtained for the sc site problem and is supported by a similar estimate, although with larger uncertainties, for the sc bond problem. It is significantly larger than (although not inconsistent with) our earlier series estimate, (2.7), of $\gamma = 1.66 \pm 0.07$, due essentially to current estimates of p_c being slightly larger than earlier estimates. Although mc estimates of γ are quite widely distributed, none of the estimates $\gamma = 1.6 \pm 0.1$ (Sur *et al* 1976), 1.8 ± 0.05 (Kirkpatrick 1976) and 1.78 ± 0.05 (Nakanishi and Stanley 1980) are inconsistent with (3.1).

The value (3.2) of β is an overall estimate obtained for *bond* percolation on *all* three-dimensional lattices. It is consistent with but more precise than earlier bond estimates, such as (1.2) and (1.4). The estimate (3.2) is a little smaller than earlier bond estimates due to increased estimates of p_c . On the other hand, (3.2) is significantly greater than earlier estimates of β , such as (1.1) and (1.3), based upon site percolation processes. The fact that the current site estimates (2.18) tend to be even smaller than the earlier site estimates is again a reflection of the increased estimates of p_c . However, the present site estimates (2.18) of β appear to be unreliable since estimates for different lattices do not exhibit universal behaviour. So far we have been unable to obtain a universal site estimate of β which is consistent with the bond estimate (3.2); this problem is being studied further.

Assuming the estimates (3.1) and (3.2), we obtain the following predictions using the standard scaling and hyperscaling laws (Stauffer 1979, Essam 1980):

$$\alpha = -0.64 \pm 0.05 \quad (3.3)$$

$$\delta = 4.81 \pm 0.14 \quad (3.4)$$

$$\Delta = 2.18 \pm 0.04 \quad (3.5)$$

$$\nu = 0.88 \pm 0.02 \quad (3.6)$$

$$\eta = 0.03 \pm 0.03. \quad (3.7)$$

The values (3.1) to (3.7) are in good agreement with the exponent set proposed by HS, namely

$$\alpha = -0.64 \quad \beta = 0.45 \quad \gamma = 1.74 \quad \delta = 4.87 \quad \nu = 0.88. \quad (3.8)$$

From (3.4) we find

$$D = d/(1 + \delta^{-1}) = 2.484 \pm 0.012 \quad (3.9)$$

for the fractal or effective dimensionality, D , of critical percolation clusters (Stauffer 1979). Note also that the uncertainties in (3.7) barely exclude the possibility of a negative value for η . Such a value does not seem impossible (de Alcantara Bonfim *et al* 1981) for although η is expected to be positive in two dimensions—hyperscaling relations plus the conjectures (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980) $\beta = \frac{5}{36}$ and $\gamma = 2\frac{7}{18}$ implying (Wu 1982) $\eta = \frac{5}{24}$ —just below the critical dimension ($d_c = 6$), it is known, from the leading term in the ϵ expansion (Amit 1976, Priest and Lubensky 1976), that η is negative.

The values of δ and Δ in (3.4) and (3.5), respectively, lie close to the centres of the ranges of values allowed by the best direct series estimates, namely $\delta = 5.0 \pm 0.8$ as in (2.20) and $\Delta = 2.2 \pm 0.1$ (Essam *et al* 1976). The value, (3.6), of ν is rather larger than the central value in many series and MC estimates, namely $\nu = 0.83 \pm 0.13$ (Skal *et al* 1975), 0.825 ± 0.05 (Dunn *et al* 1975), 0.83 ± 0.07 (Cox and Essam 1976), 0.8 ± 0.1 (Sur *et al* 1976), 0.845 ± 0.015 (Kirkpatrick 1979), ≈ 0.84 (Stauffer 1979), ≈ 0.85 (Nakanishi and Stanley 1980). However, these results are not inconsistent with (3.6) if the uncertainties (where given) are taken into account. Some of the results quoted above contain rather more detail, namely, the series estimates $\nu = 0.825 + 50\Delta p_c \pm 0.02$ ($\Delta p_c = p_c - 0.119$) and $\nu = 0.83 + 15\Delta p_c \pm 0.01$ ($\Delta p_c = p_c - 0.197$) given by Dunn *et al* (1975) and Cox and Essam (1976) for the FCC bond and site problems, respectively. Assuming the new estimates of p_c as given in (2.5) and (2.6), we find $\nu = 0.865 \pm 0.035$ and $\nu = 0.87 \pm 0.02$, respectively, in much closer agreement with (3.6). In addition, there is some MC work where the central estimates are quite close to our scaling prediction (3.6); for example, the estimate $\nu = 0.90 \pm 0.05$ of Levinshtein *et al* (1975) and, most notably, the recent estimate $\nu = 0.89 \pm 0.01$ of HS. Indeed (3.6) is identical to the value $\nu \approx 0.88$ suggested by HS as 'a good compromise'. To the best of our knowledge, there are no direct series or MC estimates of α and η with which to compare our scaling estimates (3.3) and (3.7), respectively.

There have been a number of attempts to determine the percolation exponents by RG methods. For a φ^3 field theory, expansions in $\epsilon = 6 - d$ have been computed up to order ϵ^3 (Amit 1976, Priest and Lubensky 1976, de Alcantara Bonfim *et al* 1981). However, different resummation techniques give different estimates for the critical exponents (Aharony 1980, de Alcantara Bonfim *et al* 1981) so that although all these estimates are roughly in the right region their precision is rather low. To remedy this situation attempts have been made recently to use the methods introduced by Baker *et al* (1976) and employed so successfully (Baker *et al* 1978, Le Guillou and Zinn-Justin 1977, 1980) for the φ^4 field theory. Accordingly, Fucito and Marinari (1981) have calculated the vertex functions through two loops for $d = 2, 3, 4, 5$ and their work has recently been extended (Reeve *et al* 1982) to three loops for the $d = 3$ case. In terms of the dimensionless coupling constant u , the expansions are up to order u^7 or u^6 and resummation using standard techniques gives (Reeve *et al* 1982)

$\gamma \approx 1.75$, $\eta \approx -0.16$ with $\alpha \approx -0.43$, $\beta \approx 0.34$, $\delta \approx 6.1$, $\Delta \approx 2.09$, $\nu \approx 0.81$ following from scaling. Unfortunately, the uncertainties are still expected to be quite large and Reeve *et al* feel that extension by another two loops will be required to give results comparable in accuracy to those achieved for the φ^4 model.

There has also been a great deal of work using position space renormalisation group (PSRG) methods (Stanley *et al* 1982) but most of these studies have been confined to two dimensions. For $d=3$, simple rescaling transformations have been used by several authors giving values of ν between 1.2 and 1.3 (Kirkpatrick 1977, Sarychev 1977), ≈ 1.04 (Reynolds *et al* 1977) and between 1.012 and 1.329 (Yuge 1979), compared with the expected value of $\nu \approx 0.88$. Probably the best PSRG estimates have been obtained by Burkhardt and Southern (1978) using the Kadanoff variational renormalisation transformation for the BCC lattice. They found $\alpha \approx -0.678$, $\beta \approx 0.445$, $\gamma \approx 1.79$, $\delta \approx 5.02$, $\nu \approx 0.893$ which differ from our central values, (3.1)–(3.7), by at most 6%. A similar degree of success has been obtained by Payandeh (1980) who found $\alpha \approx -0.655$, $\beta \approx 0.481$, $\gamma \approx 1.692$, $\nu \approx 0.885$, by employing a block cluster approach for the sc lattice.

Finally, we note that we have also tried analysing the same data by following different routes. For example, by using (1.5) and (1.6) to first estimate a β , assuming this to be universal and using it to obtain biased estimates of p_c for all lattices and thence biased estimates of γ . Unfortunately, this route runs into difficulties at an early stage. For the sc site problem, (1.5) gives $\beta = 0.403 \pm 0.009$ while (1.6) leads to $\beta = 0.45 \pm 0.025$ for the sc bond problem. Since these estimates do not overlap, we are unable to decide upon a universal β . This contrasts with the preferred route, followed in § 2, where (1.5) and (1.6) *did* lead to a universal γ (cf (2.1) and (2.3)). We have also tried pursuing the route followed by Sykes *et al* (1976d). Their analysis started from an estimate of $p_c = 0.119 \pm 0.001$ for the FCC bond problem. Results consistent with such an estimate have been obtained independently by a number of researchers (Sykes *et al* 1976d, Essam *et al* 1976, Dunn *et al* 1975) and it is not inconsistent with the estimate in (2.5) either. Pole-residue plots then give $\gamma = 1.66 \pm 0.11$ and adopting this as universal leads to the estimates of p_c for all other problems given by Sykes *et al* (1976d, equations (3.6) and (3.7)). Using these estimates of p_c , we find an overall estimate of $\beta = 0.474 \pm 0.014$ for bond percolation on all four lattices and $\beta = 0.40 \pm 0.035$ for site percolation on all four lattices. In contrast to the situation in § 2, therefore, estimates of β for different lattices do exhibit universal behaviour for bond *and* for site percolation. Unfortunately, the two estimates do not overlap and must be rejected as unacceptable if one insists on a universal β for both bond and site percolation.

We conclude that much series, MC and RG work remains to be done before the critical points and critical exponents associated with the standard percolation problem on three-dimensional lattices are known with the same precision and confidence as they are for the three-dimensional Ising model.

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Appendix 1. Bond percolation*Mean number*

$$K_D = 2q^6 - 2q^7 + 6q^8 - 12q^9 + 28q^{10} - 66q^{11} + 159q^{12} - 386q^{13} + 936q^{14} \\ - 2288q^{15} + 5597q^{16} - 13692q^{17} + 33448q^{18} - 81746q^{19} \\ + 199724q^{20} - 487956q^{21} + 1193006q^{22} - 2921286q^{23} \\ + 7166119q^{24} - 17620472q^{25} + \dots$$

$$K_{SC} = 3q^{10} - 3q^{11} + 15q^{14} - 30q^{15} + 18q^{16} + 65q^{18} - 225q^{19} + 288q^{20} \\ - 131q^{21} + 216q^{22} - 1272q^{23} + 2785q^{24} - 2874q^{25} + 2097q^{26} \\ - 6483q^{27} + 20265q^{28} - 34380q^{29} + 38010q^{30} - 55083q^{31} \\ + 140727q^{32} - 298438q^{33} + 453441q^{34} - 647859q^{35} \\ + 1218930q^{36} - \dots$$

$$K_{BCC} = 4q^{14} - 4q^{15} + 28q^{20} - 56q^{21} + 28q^{22} + 12q^{24} + 132q^{26} - 516q^{27} \\ + 588q^{28} - 204q^{29} + 180q^{30} - 312q^{31} + 617q^{32} - 3512q^{33} + 7332q^{34} \\ - 6008q^{35} + 3084q^{36} - 5232q^{37} + 8464q^{38} - 24904q^{39} \\ + 70903q^{40} - 99600q^{41} + 76120q^{42} - 79756q^{43} + 149582q^{44} \\ - 291432q^{45} + 695688q^{46} - 1262436q^{47} + \dots$$

$$K_{FCC} = 6q^{22} - 6q^{23} + 8q^{30} + 18q^{32} - 68q^{33} + 42q^{34} + 2q^{36} + 24q^{38} \\ - 8q^{39} + 69q^{40} - 192q^{41} + 152q^{42} - 450q^{43} + 759q^{44} - 326q^{45} + 72q^{46} \\ - 96q^{47} + 211q^{48} - 672q^{49} + 1074q^{50} - 2856q^{51} + 4353q^{52} \\ - 4596q^{53} + 8142q^{54} - 8748q^{55} + 3420q^{56} - 2872q^{57} \\ + 5568q^{58} - 9996q^{59} + 18116q^{60} - 34290q^{61} + 65796q^{62} - \dots$$

Percolation probability

$$P_D = 1 - q^6 - 6q^8 + 6q^9 - 33q^{10} + 66q^{11} - 221q^{12} + 546q^{13} - 1560q^{14} \\ + 4094q^{15} - 11160q^{16} + 29454q^{17} - 78330q^{18} + 205974q^{19} \\ - 541455q^{20} + 1414980q^{21} - 3694760q^{22} + 9628110q^{23} \\ - 25074822q^{24} + 65275798q^{25} - \dots$$

$$P_{SC} = 1 - q^{10} - 10q^{14} + 10q^{15} - 4q^{16} - 71q^{18} + 158q^{19} - 163q^{20} + 64q^{21} \\ - 402q^{22} + 1496q^{23} - 2608q^{24} + 2408q^{25} - 3347q^{26} + 11616q^{27} \\ - 28170q^{28} + 41536q^{29} - 53111q^{30} + 109460q^{31} - 265894q^{32} \\ + 491376q^{33} - 747980q^{34} + 1301370q^{35} - 2728681q^{36} + \dots$$

$$\begin{aligned}
 P_{\text{BCC}} = & 1 - q^{14} - 14q^{20} + 14q^{21} - 12q^{24} - 117q^{26} + 282q^{27} - 171q^{28} \\
 & - 234q^{30} + 288q^{31} - 806q^{32} + 3\,246q^{33} - 4\,548q^{34} + 2\,126q^{35} \\
 & - 2\,676q^{36} + 7\,014q^{37} - 10\,821q^{38} + 32\,024q^{39} - 69\,888q^{40} \\
 & + 70\,112q^{41} - 52\,406q^{42} + 108\,834q^{43} - 210\,808q^{44} + 406\,754q^{45} \\
 & - 901\,146q^{46} + 1\,331\,662q^{47} - \dots
 \end{aligned}$$

$$\begin{aligned}
 P_{\text{FCC}} = & 1 - q^{22} - 4q^{30} - 10q^{32} + 14q^{33} - 2q^{36} - 20q^{38} + 4q^{39} - 56q^{40} \\
 & + 88q^{41} - 73q^{42} + 222q^{43} - 203q^{44} - 88q^{46} + 84q^{47} - 286q^{48} + 536q^{49} \\
 & - 727q^{50} + 1\,872q^{51} - 2\,282q^{52} + 2\,586q^{53} - 4\,400q^{54} + 2\,906q^{55} \\
 & - 1\,278q^{56} + 3\,560q^{57} - 6\,076q^{58} + 11\,344q^{59} - 17\,262q^{60} \\
 & + 28\,862q^{61} - 48\,056q^{62} + \dots
 \end{aligned}$$

Susceptibility

$$\begin{aligned}
 \chi_{\text{D}} = & 2q^6 - 2q^7 + 24q^8 - 48q^9 + 222q^{10} - 594q^{11} + 2\,122q^{12} - 6\,154q^{13} \\
 & + 19\,392q^{14} - 56\,812q^{15} + 170\,272q^{16} - 492\,492q^{17} + 1\,425\,300q^{18} \\
 & - 4\,057\,284q^{19} + 11\,502\,894q^{20} - 32\,275\,770q^{21} + 90\,167\,308q^{22} \\
 & - 250\,466\,464q^{23} + 693\,280\,792q^{24} - 1\,911\,928\,816q^{25} + \dots
 \end{aligned}$$

$$\begin{aligned}
 \chi_{\text{SC}} = & 3q^{10} - 3q^{11} + 60q^{14} - 120q^{15} + 108q^{16} - 84q^{17} + 711q^{18} - 2\,109q^{19} \\
 & + 3\,381q^{20} - 3\,675q^{21} + 8\,370q^{22} - 26\,310q^{23} + 57\,072q^{24} \\
 & - 84\,648q^{25} + 132\,165q^{26} - 312\,597q^{27} + 746\,814q^{28} - 1\,377\,006q^{29} \\
 & + 2\,241\,393q^{30} - 4\,281\,693q^{31} + 9\,387\,702q^{32} - 18\,676\,398q^{33} \\
 & + 33\,057\,714q^{34} - 60\,621\,324q^{35} + 122\,743\,563q^{36} - \dots
 \end{aligned}$$

$$\begin{aligned}
 \chi_{\text{BCC}} = & 4q^{14} - 4q^{15} + 112q^{20} - 224q^{21} + 112q^{22} + 192q^{24} - 336q^{25} + 1\,692q^{26} \\
 & - 4\,980q^{27} + 5\,700q^{28} - 2\,628q^{29} + 5\,184q^{30} - 13\,032q^{31} + 27\,728q^{32} \\
 & - 77\,072q^{33} + 137\,232q^{34} - 128\,552q^{35} + 132\,656q^{36} - 290\,952q^{37} \\
 & + 562\,268q^{38} - 1\,186\,740q^{39} + 2\,461\,168q^{40} - 3\,402\,784q^{41} \\
 & + 3\,584\,672q^{42} - 5\,631\,280q^{43} + 11\,298\,752q^{44} - 21\,340\,952q^{45} \\
 & + 41\,259\,336q^{46} - 67\,922\,896q^{47} + \dots
 \end{aligned}$$

$$\begin{aligned}
 \chi_{\text{FCC}} = & 6q^{22} - 6q^{23} + 72q^{30} - 120q^{31} + 192q^{32} - 312q^{33} + 168q^{34} + 72q^{36} \\
 & - 132q^{37} + 660q^{38} - 1\,152q^{39} + 2\,112q^{40} - 4\,176q^{41} + 5\,166q^{42} \\
 & - 7\,038q^{43} + 9\,342q^{44} - 6\,534q^{45} + 5\,520q^{46} - 9\,816q^{47} + 20\,424q^{48} \\
 & - 40\,284q^{49} + 61\,794q^{50} - 102\,594q^{51} + 157\,452q^{52} - 193\,944q^{53} \\
 & + 247\,500q^{54} - 275\,820q^{55} + 251\,664q^{56} - 341\,004q^{57} + 626\,388q^{58} \\
 & - 1\,107\,552q^{59} + 1\,744\,068q^{60} - 2\,578\,416q^{61} + 3\,806\,640q^{62} - \dots
 \end{aligned}$$

Appendix 2. Site percolation*Mean number*

$$K_D = q^4 - q^5 + 2q^6 - 4q^7 + 8q^8 - 18q^9 + 40q^{10} - 82q^{11} + 153q^{12} \\ - 239q^{13} + 247q^{14} + 110q^{15} - 1492q^{16} + 5165q^{17} \\ - 13077q^{18} + 27324q^{19} - 49171q^{20} + \dots$$

$$K_{SC} = q^6 - q^7 + 3q^{10} - 6q^{11} + 3q^{12} + 12q^{13} - 33q^{14} + 35q^{15} + 16q^{16} \\ - 123q^{17} + 227q^{18} - 254q^{19} + 250q^{20} - 401q^{21} + 718q^{22} - 661q^{23} \\ - 882q^{24} + 5115q^{25} - 12597q^{26} + 22870q^{27} - 34350q^{28} + 40683q^{29} \\ - 23967q^{30} - 43037q^{31} + 191234q^{32} - 494451q^{33} + \dots$$

$$K_{BCC} = q^8 - q^9 + 4q^{14} - 8q^{15} + 4q^{16} + 12q^{17} - 36q^{18} + 48q^{19} - 2q^{20} \\ - 138q^{21} + 300q^{22} - 240q^{23} - 321q^{24} + 1298q^{25} - 1816q^{26} + 173q^{27} \\ + 4901q^{28} - 10646q^{29} + 7653q^{30} + 13440q^{31} - 45769q^{32} + 54841q^{33} \\ + 10689q^{34} - 173416q^{35} + 346809q^{36} - 259616q^{37} - 456238q^{38} \\ + 1732258q^{39} + \dots$$

$$K_{FCC} = q^{12} - q^{13} + 6q^{18} - 12q^{19} + 6q^{20} + 8q^{22} - 12q^{23} + 20q^{24} - 70q^{25} \\ + 117q^{26} - 98q^{27} + 92q^{28} - 174q^{29} + 341q^{30} - 692q^{31} + 1042q^{32} \\ - 923q^{33} + 1215q^{34} - 3724q^{35} + 7494q^{36} - 9961q^{37} + 11735q^{38} \\ - 12232q^{39} + 8142q^{40} - 13160q^{41} + 61790q^{42} - 165543q^{43} \\ + 281191q^{44} - 331658q^{45} + 251173q^{46} - 104850q^{47} + \dots$$

Percolation probability

$$P_D = 1 - q^4 - 4q^6 + 4q^7 - 18q^8 + 36q^9 - 106q^{10} + 204q^{11} - 431q^{12} \\ + 536q^{13} - 216q^{14} - 2418q^{15} + 10145q^{16} - 30378q^{17} + 70380q^{18} \\ - 140856q^{19} + 240769q^{20} + \dots$$

$$P_{SC} = 1 - q^6 - 6q^{10} + 6q^{11} - 36q^{13} + 63q^{14} - 50q^{15} - 117q^{16} + 360q^{17} \\ - 602q^{18} + 654q^{19} - 1035q^{20} + 1940q^{21} - 2789q^{22} + 354q^{23} \\ + 9425q^{24} - 32384q^{25} + 71838q^{26} - 131188q^{27} + 196124q^{28} \\ - 196560q^{29} - 22889q^{30} + 602852q^{31} - 1714585q^{32} \\ + 4104136q^{33} + \dots$$

$$P_{BCC} = 1 - q^8 - 8q^{14} + 8q^{15} - 36q^{17} + 72q^{18} - 72q^{19} - 108q^{20} + 462q^{21} \\ - 708q^{22} + 36q^{23} + 2008q^{24} - 4464q^{25} + 3545q^{26} + 6244q^{27} \\ - 25632q^{28} + 34422q^{29} + 6774q^{30} - 111432q^{31} + 203611q^{32} \\ - 106848q^{33} - 362766q^{34} + 1139334q^{35} - 1513312q^{36} \\ - 129690q^{37} + 5194415q^{38} - 10867194q^{39} + \dots$$

$$\begin{aligned}
 P_{\text{FCC}} = & 1 - q^{12} - 12q^{18} + 12q^{19} - 24q^{22} + 12q^{23} - 50q^{24} + 168q^{25} - 222q^{26} \\
 & + 140q^{27} - 252q^{28} + 558q^{29} - 1\,160q^{30} + 2\,208q^{31} - 2\,625q^{32} \\
 & + 1\,892q^{33} - 5\,372q^{34} + 16\,440q^{35} - 27\,103q^{36} + 32\,568q^{37} \\
 & - 39\,336q^{38} + 34\,236q^{39} - 15\,646q^{40} + 88\,122q^{41} - 391\,196q^{42} \\
 & + 871\,056q^{43} - 1\,268\,571q^{44} + 1\,271\,606q^{45} - 699\,941q^{46} \\
 & + 208\,512q^{47} + \dots
 \end{aligned}$$

Susceptibility

$$\begin{aligned}
 \chi_{\text{D}} = & q^4 - q^5 + 8q^6 - 16q^7 + 62q^8 - 162q^9 + 514q^{10} - 1\,162q^{11} + 2\,659q^{12} \\
 & - 3\,611q^{13} + 904q^{14} + 22\,710q^{15} - 98\,465q^{16} + 310\,895q^{17} \\
 & - 759\,348q^{18} + 1\,612\,128q^{19} - 2\,910\,657q^{20} + \dots \\
 \chi_{\text{SC}} = & q^6 - q^7 + 12q^{10} - 24q^{11} + 12q^{12} + 108q^{13} - 297q^{14} + 371q^{15} \\
 & + 277q^{16} - 1\,839q^{17} + 4\,136q^{18} - 6\,338q^{19} + 11\,067q^{20} - 20\,525q^{21} \\
 & + 30\,331q^{22} - 12\,005q^{23} - 83\,925q^{24} + 344\,823q^{25} \\
 & - 878\,610q^{26} + 1\,827\,382q^{27} - 3\,097\,608q^{28} + 3\,702\,764q^{29} \\
 & - 1\,023\,795q^{30} - 8\,111\,571q^{31} + 27\,468\,853q^{32} - 69\,643\,095q^{33} + \dots \\
 \chi_{\text{BCC}} = & q^8 - q^9 + 16q^{14} - 32q^{15} + 16q^{16} + 108q^{17} - 324q^{18} + 432q^{19} \\
 & + 276q^{20} - 2\,322q^{21} + 4\,530q^{22} - 1\,904q^{23} - 11\,226q^{24} + 31\,796q^{25} \\
 & - 33\,547q^{26} - 34\,411q^{27} + 201\,506q^{28} - 331\,014q^{29} \\
 & + 44\,214q^{30} + 951\,654q^{31} - 2\,123\,221q^{32} + 1\,619\,653q^{33} \\
 & + 3\,123\,150q^{34} - 12\,662\,446q^{35} + 20\,134\,824q^{36} - 5\,311\,154q^{37} \\
 & - 56\,990\,251q^{38} + 146\,757\,109q^{39} + \dots \\
 \chi_{\text{FCC}} = & q^{12} - q^{13} + 24q^{18} - 48q^{19} + 24q^{20} + 72q^{22} - 108q^{23} + 194q^{24} \\
 & - 686q^{25} + 1\,326q^{26} - 1\,358q^{27} + 1\,688q^{28} - 3\,810q^{29} + 8\,654q^{30} \\
 & - 16\,496q^{31} + 22\,839q^{32} - 22\,901q^{33} + 43\,426q^{34} - 127\,100q^{35} \\
 & + 252\,597q^{36} - 356\,903q^{37} + 439\,070q^{38} - 435\,448q^{39} + 295\,530q^{40} \\
 & - 809\,096q^{41} + 3\,730\,382q^{42} - 9\,682\,820q^{43} + 16\,416\,315q^{44} \\
 & - 19\,719\,905q^{45} + 15\,692\,023q^{46} - 7\,436\,369q^{47} + \dots
 \end{aligned}$$

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