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Estimation of critical indices for the three-dimensional Ising model

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Abstract. New series expansion data for the three-dimensional Ising model are analysed. A special study of the diamond and face-centred cubic lattices is made. Below the critical temperature convergence is found to be slow. It is concluded that all available data are consistent with $\beta = \frac{5}{16}$ (magnetization) and not inconsistent with the 'scaling' value $\gamma' = 1\frac{1}{4}$ (susceptibility) and that with the data and methods available at present it is not possible to draw more precise conclusions.

1. Introduction

It is the main purpose of this paper to examine new data for the Ising model on the face-centred cubic and diamond lattices. We study the critical indices for the zero-field specific heat C_H and reduced susceptibility χ above (α, γ) and below (α', γ') the critical temperature T_c, and for the spontaneous magnetization $I(\beta)$. The precise determination of these indices is of great theoretical interest; they are of particular relevance to the theory of scaling. (For a general introduction and review see Domb 1960 and Fisher 1963, 1965, 1967; for series analysis techniques see Gaunt and Guttmann 1973; for the theory of scaling see Fisher 1967, Kadanoff *et al* 1967 and Stanley 1971).

Recently extended data for the high-temperature expansions of the specific heat and susceptibility of the face-centred, body-centred and simple cubic lattices appear to be quite consistent with the long-held view that the critical indices α and γ are exactly $\frac{1}{8}$ and $1\frac{1}{4}$ respectively, in three dimensions (Sykes *et al* 1972a, b, c); further the decay of even–odd oscillations for the body-centred and simple cubic lattices is consistent with the independent direct estimates of the critical specific heat index (Sykes *et al* 1972b, c).

In figure 1 we illustrate what may be described as the orthodox view of the high-temperature situation. Using expansions in powers of the standard high-temperature counting variable $v = \tanh K$:

$$\chi = \sum a_n v^n \tag{1.1}$$

$$\frac{C_H}{R} = \sum b_n v^n, \tag{1.2}$$

ratios of successive coefficients for the face-centred cubic lattice are plotted against $1/n$. It will be seen that the behaviour exhibits a striking linearity for quite small values of n; similar results are obtained for the simple cubic lattice and body-centred cubic lattice which exhibit an even–odd oscillation. The development of a regular pattern of behavior for small values of n is an observed fact; the implicit assumption of the method is

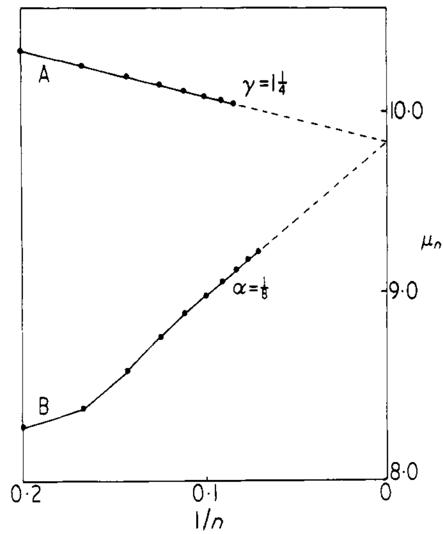

Figure 1. High-temperature situation for the face-centred cubic lattice. Ratios μ_n of successive coefficients of the zero-field susceptibility (A) and specific heat (B) series plotted against $1/n$. The asymptotes corresponding to $\gamma = 1\frac{1}{4}$ and $\alpha = \frac{1}{8}$ with $1/v_c = 9{\cdot}8290$ (Sykes *et al* 1972b) are shown as broken lines.

that the hypotheses made to explain this behaviour (the presence of the singularities described in detail by Sykes *et al* 1972a, b, c) are correct and that the extrapolation represented by the broken lines is essentially valid. On this basis precise estimates of the critical temperature can be made (Sykes *et al* 1972b). Loose-packed lattices of low coordination number present a more complex situation; there seems no reason to doubt, however, that the dominant singularities remain the same. We examine this aspect in § 2 since we require an estimate of the critical temperature of the diamond lattice.

In contrast to the simple high-temperature situation depicted in figure 1 the face-centred cubic lattice yields low-temperature expansions with a most irregular pattern, the extrapolation of which long presented a problem; the coefficients can be regrouped (Domb and Sykes 1956) but it appears better to resort to more general methods of extrapolation (see Gaunt and Guttmann 1973).

Expansions for the spontaneous magnetization and zero-field configurational free energy in powers of $u = \exp(-4J/kT)$ are given by Sykes *et al* (1965), and for the zero-field susceptibility by Essam and Fisher (1963), through u^{28}; recently these expansions have been extended by specialized techniques (Sykes *et al* 1973c, d, e) through u^{40} (Sykes *et al* 1973a, b) and we make an analysis of the new data in § 3. Loose-packed lattices of low coordination number appear to present a less complex situation; it was suggested by Block (1963) that the diamond lattice be studied as it seemed to give series whose coefficients are all of one sign and should therefore converge up to the critical temperature; this property was confirmed by the investigation of Essam and Sykes (1963) who derived expansions through u^{12}. These expansions are now available through u^{15} (Sykes *et al* 1973a, b).

In figure 2 we illustrate the ratio plot which corresponds to the present low-temperature situation on the diamond lattice. The susceptibility is less well behaved than most high-temperature expansions but appears to be settling down, with an asymptote

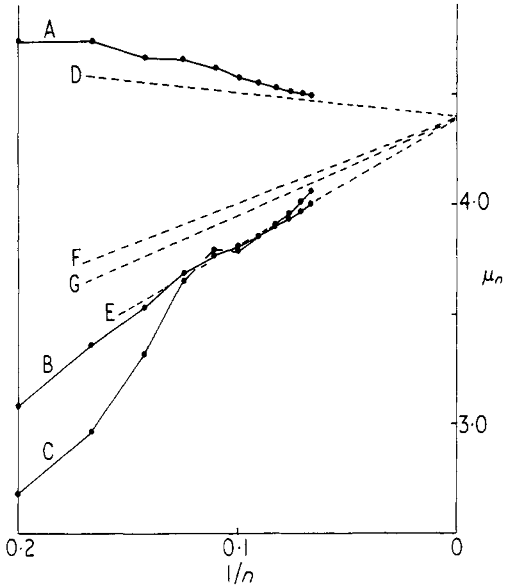

Figure 2. Low-temperature situation for the diamond lattice. Ratios μ_n of successive coefficients of the zero-field susceptibility (A), magnetization (B) and specific heat (C) series plotted against $1/n$. The asymptotes corresponding to $\gamma' = 1\frac{1}{4}$ (D), $\beta = \frac{5}{16}$ (E), $\alpha' = \frac{1}{8}$ (F) and $\alpha' = 0$ (G) with $1/v_c = 2{\cdot}8264$ (equation (2.6)) are shown as broken lines.

corresponding to $\gamma' = 1\frac{1}{4}$ or alternatively perhaps as much as 10% above this. The magnetization expansion is also apparently converging with an asymptote close to $\beta = \frac{5}{16}$. Even with $n = 15$, however, the specific heat can hardly be said to have converged and is still quite consistent with $\alpha' = \frac{1}{8}$ or $\alpha' = 0$ (logarithm). The situation is closely analogous to the high-temperature situation of figure 1 where the specific heat only becomes smooth for higher values of n than the susceptibility. We conclude from figure 2 that altogether the general quality of the data is still much inferior to that available at high temperatures. It is possible the situation could be improved by choosing still looser packed lattices, such as the hydrogen peroxide lattice (Leu *et al* 1969) and this possibility is currently being investigated (Betts, private communication).

2. Estimation of the critical point for the diamond lattice

The critical temperature of a three-dimensional lattice is usually estimated from the high-temperature expansion of the susceptibility; to provide guidelines to the asymptotic behaviour the most nearly related two-dimensional lattice whose critical temperature is known is usefully studied at the same time (Sykes *et al* 1972a, b). For the diamond lattice we therefore examine the honeycomb lattice; unfortunately, as is well known, this lattice has a susceptibility expansion whose behaviour is complicated by the apparent presence of a pair of complex conjugate singularities on the radius of convergence, lying on the imaginary axis (Sykes and Fisher 1962, Sykes *et al* 1972a). This makes the refined analyses developed for other lattices (Sykes *et al* 1972b) less effective; in a previous investigation (Sykes *et al* 1972a) we have been unable to provide a completely satisfactory representation for the honeycomb susceptibility. However this does not mean that the series cannot be made to yield satisfactory estimates of the critical temperature; for this it suffices to seek empirical methods of averaging or smoothing the oscillations.

Essam and Sykes (1963) in their study of the diamond lattice give the susceptibility expansion in the form (1.1) through v^{16}. We have corrected a small error in the last coefficient and extended the series through v^{22} to obtain:

$$\begin{aligned}\chi = {} & 1+4v+12v^2+36v^3+108v^4+324v^5+948v^6+2772v^7+8076v^8+23508v^9 \\ & +67980v^{10}+196548v^{11}+566820v^{12}+1633956v^{13}+4697412v^{14} \\ & +13501492v^{15}+38742652v^{16}+111146820v^{17}+318390684v^{18} \\ & +911904996v^{19}+2608952940v^{20}+7463042916v^{21}+21328259716v^{22} \\ & +\dots\end{aligned} \tag{2.1}$$

Essam and Sykes used the quantities

$$\beta_n = \left(\frac{na_n}{a_{n-1}}\right)(n+\gamma-1)^{-1} \tag{2.2}$$

$$\bar{\beta}_n = \tfrac{1}{2}(\beta_n+\beta_{n-1}) \tag{2.3}$$

the latter average being introduced to smooth even–odd oscillations. In figure 3 we illustrate these quantities for the honeycomb lattice. Both β and $\bar{\beta}$ exhibit an oscillation of period four which corresponds to the interplay of an even–odd oscillation (due to the antiferromagnetic singularity) and an oscillation usually ascribed to the pair of complex conjugate singularities on the imaginary axis. The quantity $\bar{\beta}$ does not represent any noticeable improvement on β; this is because for the honeycomb, the pair of singularities on the imaginary axis is at least comparable in strength with the antiferromagnetic singularity. However $\bar{\beta}$ contains a subsequence (n even) which approaches the exact limit (1·7320508...) fairly smoothly. From figure 3

$$1/v_c = 1{\cdot}731 \pm 0{\cdot}004 \tag{2.4}$$

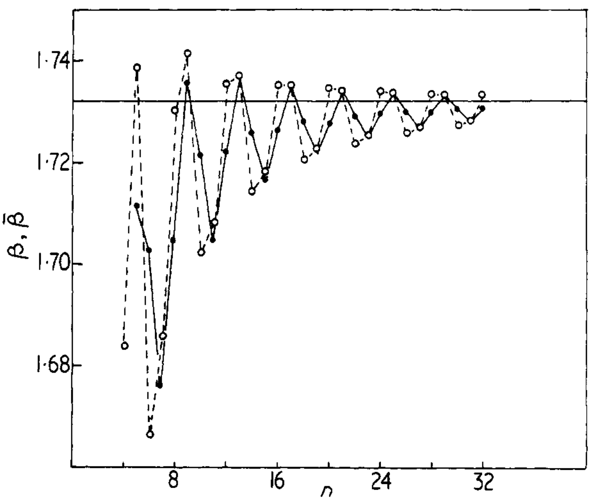

Figure 3. Honeycomb lattice. Plots against n of successive estimates for $1/v_c$ provided by β_n (broken lines) and $\bar{\beta}_n$ (full lines). The horizontal line represents the exact limit.

would seem a not unreasonable objective estimate; it represents an uncertainty of about $\frac{1}{4}\%$. Figure 3 also well illustrates the fact that by a study of β the dominant ferromagnetic singularity is allowed for, and the remaining irregularities cluster around the true limit which is approached more or less symmetrically.

In figure 4 we illustrate the same quantities for the diamond lattice. The general conclusion of Essam and Sykes (1963) that the terms then available had settled down to a characteristic even–odd oscillation (in β) is still consistent with the behaviour of the six new coefficients. The troublesome oscillation of period four which is present in the honeycomb was not noticed for the diamond; it will be seen from figure 4 that there is

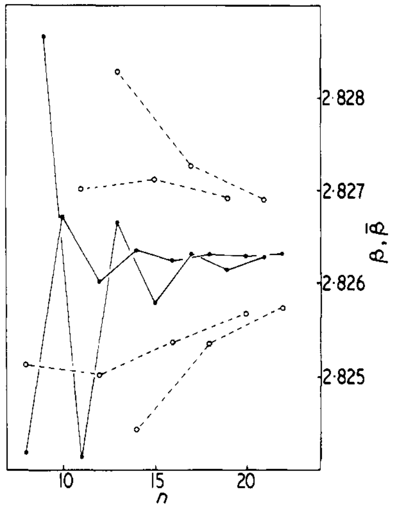

Figure 4. Diamond lattice. Plots against n of successive estimates for $1/v_c$ provided by β_n (broken lines) and $\bar{\beta}_n$ (full lines).

now some evidence that an oscillation of this kind is becoming established; its amplitude appears to be much less than that of the dominant even–odd oscillation, which latter can be understood in the usual way as due to the antiferromagnetic singularity. It is to be supposed that here also there is a conjugate pair of singularities on, or very close to, the radius of convergence and the imaginary axis. This has been confirmed by a Padé approximant analysis of the $(d/dv) \ln \chi(v)$ series.

The new data are quite consistent with the 1963 estimate of

$$1/v_c = 2{\cdot}8262 \pm 0{\cdot}0005 \tag{2.5}$$

but if the indicated trend continues then we would conclude that the limit is very slightly higher at

$$1/v_c = 2{\cdot}8264 \pm 0{\cdot}0002 \tag{2.6}$$

which is included in (2.5). A more refined study is difficult because it requires some hypothesis about the nature of the generating function corresponding to the period four oscillation; as we have seen this has not proved possible for the honeycomb lattice. Fortunately the disturbing singularities seem to be less violent in their effect and the estimate (2.6) should be a reasonable one subject to the assumptions of the method.

Although ten fewer coefficients are available the oscillations are about a tenth as large making (2.6) correspondingly more precise than (2.4).

The ratio method is particularly sensitive to small deviations from the assumed asymptotic behaviour. For the situation depicted in figure 1 this is all to the good, since the convergence is then seen to be all the more impressive. However, when the asymptotic behaviour is perturbed by contributions from interfering singularities lying on, or close to, the circle of convergence, we would expect the Padé approximant procedures to be more suitable. This is supported by the numerical experiments of Hunter and Baker (1973) for a variety of test functions. We present in table 1 diagonal and paradiagonal sequences of Padé approximant estimates of $1/v_c$ for the honeycomb and diamond lattices. These were obtained by calculating the reciprocals of the appropriate poles of Padé approximants to the series expansions of $(\chi(v))^{1/\gamma}$. For the honeycomb lattice the last few estimates in each sequence differ from the exact result by less than 7 parts in 10^6; this represents a substantial increase in accuracy over (2.4). For the diamond lattice the sequences appear to be converging just as rapidly and we estimate

$$1/v_c = 2{\cdot}82641 \pm 0{\cdot}00010 \tag{2.7}$$

in excellent agreement with (2.6) and some two times as precise.

Table 1. Honeycomb and diamond lattices. Estimates of $1/v_c$ provided by the $[n+j/n]$ Padé approximants. 'Defective' approximants having a 'spurious' pole with very small residue on the positive (†) and negative (‡) real axes, and in the complex plane (§) are indicated.

	Honeycomb			Diamond		
$n \backslash j$	−1	0	+1	−1	0	+1
1	1·714	1·357	1·729	3·200	2·600	2·785
2	1·529	1·758	1·712†	2·736	2·858	2·932
3	1·858	1·775‡	1·750§	2·912	2·865‡	2·833
4	1·697	1·717	1·725	2·824	2·825	2·826706
5	1·737	1·731073	1·734	2·840	2·826568	2·826321
6	1·732567	1·732529	1·732205	1·826479	2·826828†	2·826130‡
7	1·732574†	1·732063	1·732077	2·826398	2·826413	2·826421
8	1·732078	1·732063‡	1·732810†‡	2·826430	2·826418	2·826418
9	1·731814‡	1·731979§	1·732061‡§	2·826418	2·826418†	2·826420†
10	1·732186§	1·732074§	1·732067§§	2·826420†	2·826417§	2·826394
11	1·732059	1·732057	1·732047	2·826408§	2·826488†	
12	1·732060†	1·732030	1·732041			
13	1·732045	1·732042	1·732040†			
14	1·732044‡	1·732048‡	1·732045			
15	1·732045	1·732045	1·732047			
16	1·732045†	1·732046				

3. Analysis of low-temperature series

Using the ratio method we may try to estimate the index γ' for the diamond lattice from the sequence

$$\gamma'_n = 1 + n\left(u_c \frac{a_n}{a_{n-1}} - 1\right) \tag{3.1}$$

where now a_n is the coefficient of u^n in the low-temperature expansion of $\chi(u)$, and $u_c = \exp(-4J/kT_c)$ is calculated from the central value in (2.6). Successive estimates are plotted against $1/n$ in figure 5. We have repeated the calculations using the largest and smallest values of $1/v_c$ allowed by the uncertainties in (2.6); the upper end of the error bar in figure 5 corresponds to the largest value, and vice versa. It is evidently not possible to attribute the 'hook' which develops in figure 5 for $n > 13$ to uncertainties in the critical temperature.

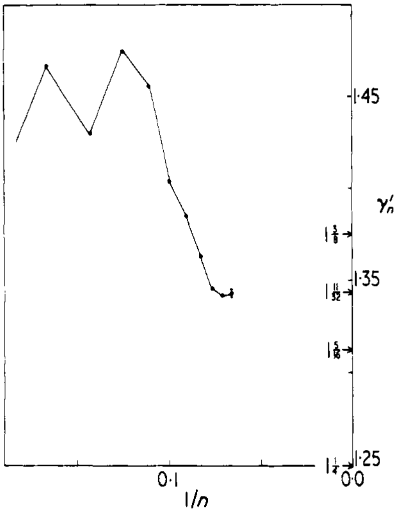

Figure 5. Diamond lattice. Plots against $1/n$ of successive estimates for γ' provided by γ'_n. The error bar corresponds to the uncertainties in the critical temperature. For $n < 15$ the errors are even smaller.

Without the last two coefficients it might be thought that the series had settled down, suggesting a limit close to $1\frac{1}{4}$; apparently this is not the case. However we do not think that the 'hook' necessarily excludes $1\frac{1}{4}$ (or $1\frac{5}{16}$, or any other value for that matter) from being the exact limit; it simply implies that the series has still not settled down to its asymptotic behaviour. It seems likely that the slow convergence is related to the presence of disturbing singularities. A Padé approximant analysis of the $(\mathrm{d}/\mathrm{d}u) \ln \chi(u)$ series reveals a (complex conjugate) pair of non-physical singularities at

$$u^* = (-0{\cdot}20 \pm 0{\cdot}20\mathrm{i}) \pm (0{\cdot}04 \pm 0{\cdot}03\mathrm{i}). \tag{3.2}$$

Since $|u^*|/u_c = 1{\cdot}23 \pm 0{\cdot}23$, these lie just outside (or possibly on) the radius of convergence $|u| = u_c = 0{\cdot}22783\ldots$.

Following Essam and Sykes (1963), we study the index β for the diamond lattice by examining the series for

$$-u\frac{\mathrm{d}}{\mathrm{d}u} \ln I(u) = \sum_{n=2}^{\infty} c_n u^n. \tag{3.3}$$

If near u_c

$$I(u) \sim B(u_c - u)^{\beta} \tag{3.4}$$

where B is a constant amplitude, then it is easily shown that

$$c_n \sim \frac{\beta}{u_c^n} \qquad (n \to \infty). \tag{3.5}$$

We have calculated successive estimates, $c_n u_c^n$, for β and find

$$\ldots 0{\cdot}30338, 0{\cdot}30619, 0{\cdot}30742, 0{\cdot}30849, 0{\cdot}30924, 0{\cdot}30974, 0{\cdot}31027, 0{\cdot}31088. \tag{3.6}$$

(Uncertainties in u_c only affect the fourth decimal place.) The sequence is increasing slowly and is quite consistent with $\beta = \frac{5}{16}$; however the situation is closely analogous to that which obtains for the low-temperature susceptibility, in that the estimates are not sufficiently smooth to be extrapolable against $1/n$.

Finally we try a Padé approximant analysis of the $\chi(u)$ and $I(u)$ series for both the diamond and face-centred cubic lattices. In view of the interfering singularities (3.2), the Padé approximant method may well be preferable to the ratio and related techniques used above for the diamond lattice; this follows from the discussion of § 2. For the face-centred cubic lattice the ratio method is not applicable and the Padé approximant technique is the obvious choice. Although in one sense this lattice is the most difficult case by virtue of four non-physical singularities lying inside the circle $|u| = u_c$ (Guttmann 1969), on the other hand the series are known further than for any other lattice.

Estimates for γ' and β are presented in table 2 and were obtained in the usual way by evaluating Pade approximants to the $(u_c - u)(\mathrm{d}/\mathrm{d}u) \ln \chi(u)$ and $(u - u_c)(\mathrm{d}/\mathrm{d}u) \ln I(u)$ series respectively, at $u = u_c$. The results certainly suggest that β is the same for both lattices and yield the estimate

$$0{\cdot}307 \leqslant \beta \leqslant 0{\cdot}317 \tag{3.7}$$

in support of the conjecture $\beta = \frac{5}{16}$. Comparable results are obtained for the body-centred and simple cubic lattices. The last few estimates of γ' for the face-centred cubic lattice (excluding those approximants with 'defects', see Gaunt and Guttmann 1973) lie between 1·27 and 1·28. For the diamond lattice, the estimates tend to be somewhat larger and are mostly centred around 1·30. The corresponding results for the body-centred cubic lattice are similar to those for the face-centred cubic lattice; those for the simple cubic lattice are closer to those for the diamond lattice. Since we believe the index γ' to be the same for all these three-dimensional lattices, we conclude that the rate of convergence is too slow for precise conclusions to be drawn. However we consider the data justify our interpretation of figure 5; none of the results are necessarily inconsistent with the scaling value $\gamma' = 1\frac{1}{4}$.

4. General conclusions

We have presented an analysis of new low-temperature series expansion data for the spontaneous magnetization and zero-field susceptibility of the Ising model for three-dimensional lattices. Although the diamond lattice yields expansions whose coefficients are all of one sign, and whose radius of convergence can be presumed accurately known from the high-temperature susceptibility expansion, convergence has been found disappointingly slow especially for the susceptibility series. Padé approximant studies of the corresponding series for the face-centred cubic lattice seem reasonably convergent for β but are inconclusive for γ'. We are of the opinion that the only reasonable conclusion

Table 2. (*a*) Diamond and (*b*) face-centred cubic lattices. Estimates of γ' and β provided by the $[n+j/n]$ Padé approximants. The uncertainties in u_c affect the last decimal place of the γ' and β estimates by no more than 2 and 6 respectively. 'Defective' approximants having a 'spurious' pole with very small residue on the positive (†) and negative (‡) real axes are indicated.

	γ'				β		
$n \backslash j$	−1	0	+1	$n \backslash j$	−1	0	+1
(*a*) Diamond							
1	1·384	0·622	1·147	1		0·3280	0·3073
2	1·241	1·261	1·330	2	0·3048	0	0·2967
3	1·225†	1·415	1·347	3	0·2944‡	0·2985	0·2937†
4	1·294	1·313	1·308	4	0·3066	1·3646	0·3016
5	1·309	1·316†	1·269	5	0·3142	0·3100	0·3115
6	1·297	1·292		6	0·3110	0·3112	0·3114‡
7				7	0·3107†	0·3110†	
(*b*) Face-centred cubic							
5	1·305	0·754	1·200	8	0·2983	0·3050‡	0·3077
6	1·206	2·437†	1·254	9	0·3073	0·3071	0·3074
7	1·260	1·252	1·255†	10	0·3073‡	0·3085	0·3089
8	1·287†	1·244	1·248	11	0·3089	0·3085†	0·3061†
9	1·249	1·263	1·236†	12	0·3056†	0·3058†	0·3061†‡
10	1·240†	1·362	1·334	13	0·3055††	0·3063†	0·3061†
11	1·334	1·355‡	1·352‡	14	0·3059†	0·3051†	0·3779
12	1·352‡	1·355†‡	1·271	15	0·3081	0·3061††	0·3095‡
13	1·274	1·274	1·257†	16	0·3074‡	0·3156‡	0·3129
14	1·274‡	1·275	1·277‡	17	0·3126	0·3139	0·3112†
15	1·324‡	1·272†‡	1·280	18	0·3043†	0·3164	0·3164
16	1·256†‡‡	1·278	1·319†	19	0·3164	0·3164‡	
17	1·276						

that can be drawn by present methods from the data available is that it is quite consistent with $\beta = \frac{5}{16}$ and not inconsistent with $\gamma' = 1\frac{1}{4}$. We are deriving further coefficients in an attempt to resolve the uncertainty on γ'.

Acknowledgments

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