High temperature series for the susceptibility of the Ising model. II. Three dimensional lattices



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# High temperature series for the susceptibility of the Ising model II. Three dimensional lattices

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**Abstract.** Extended series expansions for the high temperature zero-field susceptibility of the Ising model are given in powers of the usual high temperature counting variable $v = \tanh K$ for the simple cubic lattice to $v^{17}$, the body-centred cubic lattice to $v^{15}$, and the face-centred cubic lattice to $v^{12}$, inclusive. The coefficients are analysed by the ratio method and it is estimated that, subject to the implicit assumptions thereof, the critical temperatures correspond to $v_f = 0{\cdot}21813 \pm 0{\cdot}00001$ (SC), $v_f = 0{\cdot}15612 \pm 0{\cdot}00003$ (BCC) and $v_f = 0{\cdot}10174 \pm 0{\cdot}00001$ (FCC). The asymptotic behaviour of the coefficients is studied in detail; for the loose-packed lattices the decay of the even–odd oscillation in the ratios is found to be consistent with the assumption that the critical index of the high temperature specific heat is very close to $\frac{1}{8}$.

## 1. Introduction

Exact series expansions have been widely used to study the physical properties of the three dimensional Ising model of a ferromagnet and an antiferromagnet. There is an extensive literature and we shall assume a general familiarity with the problem; reviews on a broad base are those of Domb (1960), Fisher (1967), and Kadanoff *et al* (1967). In a previous paper (Sykes *et al* 1972a, to be referred to as I) we have given a specialized introduction to a study of the susceptibility of the two dimensional Ising model; this paper studies the analogous problem presented by the three dimensional Ising model. We follow the notation of I.

In I we extended series expansions for the susceptibility in two dimensions and found that the second order asymptotic behaviour, or approach terms, can apparently be recognized. In this paper we present extended series expansions for the susceptibility of some three dimensional lattices. We have derived expansions for the reduced zero-field susceptibility in ascending powers of the high temperature counting variable $v = \tanh K$ in the form

$$\chi = \sum_{r=0}^{\infty} a_r v^r \qquad a_0 = 1. \tag{1.1}$$

We have extended the expansions for the simple cubic lattice by six coefficients to $v^{17}$, for the body-centred cubic lattice by six coefficients to $v^{15}$, and for the face-centred cubic lattice by four coefficients to $v^{12}$. We give these expansions in the Appendix; as in I, and for the same reasons, we do not describe the derivation. We present the

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investigation in the variable $v$ only, as we have found the extrapolations quite insensitive to a change to the more direct temperature scale that corresponds to using $K$ in place of tanh $K$.

The ferromagnet exhibits a phase transition at a critical temperature $T_C$ and much effort has been devoted to an elucidation of the critical behaviour of the physical properties near $T_C$. The most successful general approach appears to be that of exact series expansions. In general it has been found that series expansions above $T_C$ are reasonably well behaved and converge right down to the critical point; in other words the radius of convergence of high temperature expansions determines $T_C$. In contrast, series expansions below $T_C$ are usually ill behaved and do not converge up to the critical point. Such behaviour is apparently due to nonphysical singularities in the complex plane, inside the physical disc $|T| \leqslant T_C$; when, exceptionally, the series do converge up to the critical point their behaviour is not as good as at high temperatures (Essam and Sykes 1963).

To exploit a series expansion effectively, an accurate estimate of the radius of convergence is required. For high temperature series it is customary to assume that estimates derived from the high temperature susceptibility expansion are the most precise, and in general these are adopted in studies of critical behaviour (Essam and Fisher 1963). However the practical estimation of the radius of convergence of a power series usually involves making assumptions about its generating function; in some instances this could give rise to cyclical argument and result in errors of interpretation. Fortunately, for the physical properties of interest, such as susceptibility and specific heat, it seems that the dominant, or first order, critical behaviour above $T_C$ is reasonably well indicated.

In the critical region for a ferromagnet the reduced susceptibility is found to behave asymptotically as

$$\chi \sim A_{\pm}(1-v/v_f)^{-1\cdot 25} \qquad v \to v_f \mp \tag{1.2}$$

where $v_f = \tanh J/kT_C$, and the amplitudes $A_+$ and $A_-$ above and below the critical temperature $T_C$ are constants. The form (1.2) differs from that found in two dimensions only in the value of the critical index of 1·25 in place of 1·75. Originally based on series expansions (Domb and Sykes 1957), the conjecture for three dimensions is reasonably consistent with the available data and is appealingly simple. We investigate higher order terms in the asymptotic expansion (1.2) above $T_C$. We find that, in close analogy with the two dimensional result, the data are consistent with the form

$$\chi \sim (1-v/v_f)^{-1\cdot 25}\Phi(v)+\Psi(v) \tag{1.3}$$

where $\Phi$ is regular in the disc $|v| \leqslant v_f$ and $\Psi$ is not singular at $v = v_f$. The amplitude $A_+ = \Phi(v_f)$ but $\Psi(v_f) \neq 0$ although the ratio $\Psi(v_f)/\Phi(v_f)$ is small; this latter finding accounts for the reasonable success of earlier investigations based on dividing out the dominant singularity (Fisher and Sykes 1962).

In the antiferromagnetic critical region for a loose-packed lattice the reduced susceptibility, following the general arguments of I, is expected to behave like the energy. Fisher and Sykes (1962) followed Wakefield (1951) in assuming a logarithmic singularity in the specific heat and the corresponding form

$$\chi \sim \chi_a - a_{\pm}(1+v/v_f)\ln|1+v/v_f| \qquad v \to v_a = -v_f. \tag{1.4}$$

More recent investigations (Sykes *et al* 1967 and 1972b) have suggested that the specific heat above $T_C$ is not logarithmic but instead diverges inversely as an one eighth power; the corresponding form is

$$\chi \sim \chi_a + a_+(1+v/v_f)^{0\cdot 875} \qquad v \to -v_f+. \tag{1.5}$$

We shall find the extended data consistent with this assumption.

The general scheme of our treatment is first to seek guidelines by an analysis of the coefficients in expansions for two dimensional lattices where the radius of convergence is known; then we investigate whether a similar pattern of asymptotic behaviour can be recognized in the coefficients in expansions for three dimensional lattices. We anticipate our conclusions and state that we believe it can; on this basis we make what we consider to be precise estimates of critical temperatures subject to the implicit assumptions and hypotheses of the method.

## 2. Close-packed lattices

The elementary treatment (Domb and Sykes 1957) supposes that near $T_C$

$$\chi \sim A(1-\mu v)^{-\gamma} \qquad \mu = \frac{1}{v_f} \qquad v \to v_f- \tag{2.1}$$

where $A$ (the amplitude) and $\gamma$ (the critical index) are constants. It follows from the binomial theorem that the ratio of successive coefficients in the expansion of the susceptibility satisfies

$$\mu_n = \frac{a_n}{a_{n-1}} \sim \mu\left(1+\frac{\gamma-1}{n}\right). \tag{2.2}$$

In words: as $n$ increases, $\mu_n$ *should approach linearity against* $1/n$. The parameters $\mu$ and $\gamma$ can be estimated by plotting the available values of $\mu_n$ against $1/n$ and extrapolating graphically, or by equivalent numerical procedures. Early studies suggested strongly that the critical index is insensitive to the structure of the lattice and very close to 1·75 in two dimensions and 1·25 in three dimensions. By making the hypothesis that these appealingly simple fractions are exact more precise estimates of $\mu$ (consistent with the hypothesis) can be made. This is conveniently done (Domb and Sykes 1961) by assuming $\gamma$ in (2.1) and studying

$$\beta_n = \frac{n\mu_n}{n+\gamma-1} \tag{2.3}$$

which, from (2.1), should approach $\mu$ with no slope against $1/n$. Now that longer series are available it is worthwhile extending the treatment to higher order. Following I we replace (2.1) by the more general assumption that near $T_C$

$$\chi \sim (1-\mu v)^{-\gamma}\Phi(v)+\Psi(v) \tag{2.4}$$

where $\Phi$ and $\Psi$ are regular in the disc $|v| \leqslant v_f$. The corresponding asymptotic behaviour of $\beta_n$ is readily derived from the analysis of I (equation (2.5)) and we find

$$\beta_n = \mu\left(1+\frac{\xi}{n^2}+\frac{\xi^*}{n^3}+\frac{\xi^{**}}{n^4}+\dots\right) \tag{2.5}$$

where $\xi$, $\xi^*$,... are constants. In words: as $n$ increases, $\beta_n$ *should approach linearity against* $1/n^2$. More generally $\beta_n$ should be represented by an expansion in inverse powers of $n$. Attempts to fit numerical data to representations of this kind are notoriously difficult when only a few terms are available and often give rise to so called small number effects. We investigate the possibility for the triangular lattice by solving two orders of approximation (to the ferromagnetic singularity).

First order, which we denote by $\beta(1\text{F})$

$$\beta_n = \mu\left(1+\frac{\xi}{n^2}\right). \tag{2.6}$$

Second order, which we denote by $\beta(2\text{F})$

$$\beta_n = \mu\left(1+\frac{\xi}{n^2}+\frac{\xi^*}{n^3}\right). \tag{2.7}$$

The procedure is to solve (2.6) using successive pairs, or (2.7) using successive triplets, of $\beta_n$ and so obtain a sequence of estimates for $\mu$. We illustrate the results in figure 1.

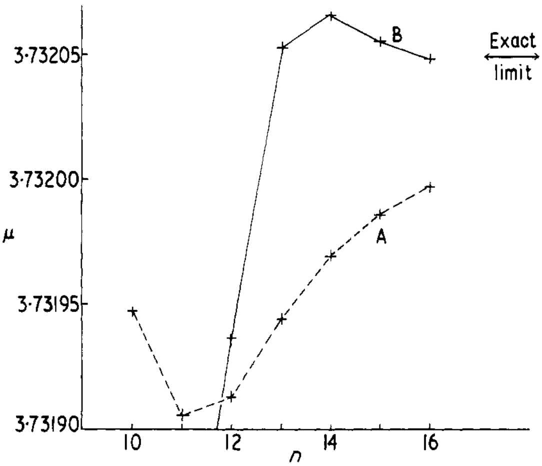


**Figure 1.** Triangular lattice. Estimates for $\mu = 1/v_c$. (A) First order approximation $\beta(1\text{F})$. (B) Second order approximation $\beta(2\text{F})$.

It is clear that only after about a dozen terms does any definite trend develop. For the higher terms available the first order approximation settles down to a smooth sequence of estimates for the critical point; the second order approximation appears to be on the verge of becoming smooth. The last estimate of $\beta(1\text{F})$ is within 1 part in 50 000 of the correct value, that of $\beta(2\text{F})$ within 1 part in 200 000.

The fact that the asymptotic forms fit the data for two dimensions well is only to be expected from the investigation of I; the limiting asymptotic behaviour there proposed (I, (2.6)) corresponds to

$$\chi \sim A(1-\mu v)^{-\gamma}+B(1-\mu v)^{-\gamma+1}+C(1-\mu v)^{-\gamma+2}+\ldots+\Psi(v) \tag{2.8}$$

with $\gamma = 1{\cdot}75$ and $A, B, C,\ldots$ constants which can be related to $\xi$, $\xi^*$,... of (2.5). In particular

$$\xi = \frac{-(\gamma-1)B}{A}. \tag{2.9}$$

From the data illustrated in figure 1 we conclude that the proposed sequence of approximations provides a satisfactory procedure for locating the critical point. With the data presently available no improvement results from approximations of higher order than (2.7).

For the face-centred cubic lattice we now try the assumption that (2.8) still holds with $\gamma = 1{\cdot}25$. We illustrate the corresponding results for $\beta(1\mathrm{F})$ and $\beta(2\mathrm{F})$ in figure 2.

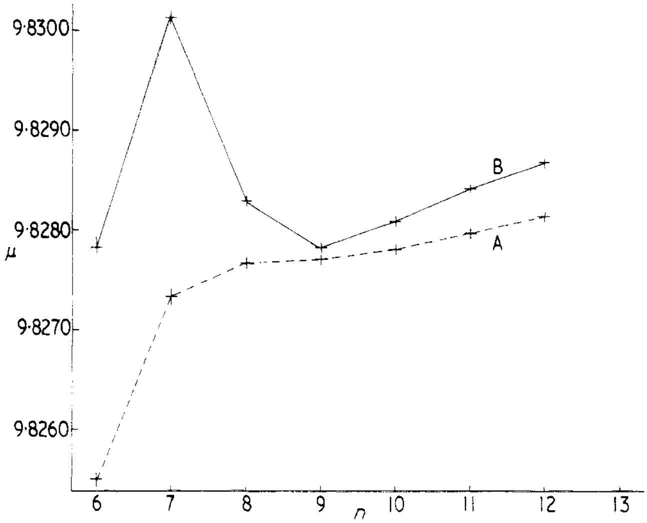


**Figure 2.** Face-centred cubic lattice. Estimates for $\mu = 1/v_c$. (A) First order approximation $\beta(1\mathrm{F})$. (B) Second order approximation $\beta(2\mathrm{F})$.

In assessing these it should be realized that only 12 coefficients are available; therefore, unless convergence is much more rapid in three dimensions, a smooth region should barely have been reached; in addition the asymptotic behaviour might well be more complex. Nevertheless we consider the results consistent with the view that a steady behaviour is developing and make the estimate

$$\mu = 9{\cdot}8290 \pm 0{\cdot}0005. \tag{2.10}$$

Further coefficients are needed to confirm that the indicated trends persist; the estimate (2.10) assumes they do. So far we have found nothing inconsistent with the hypothesis that (2.8) is applicable in three dimensions.

Because of the limited data we do not present a detailed analysis. Following the method of I (§ 2) the available coefficients can be fitted to (2.8) to give an approximate representation consistent with (2.10). Writing $t = v/v_f$ we obtain (correct to 4 decimal places)

$$\chi(v) \simeq 0{\cdot}9634(1-t)^{-1{\cdot}25} + 0{\cdot}1965(1-t)^{-0{\cdot}25} + 0{\cdot}4993(1-t)^{0{\cdot}75} + \Psi_3(t) \tag{2.11}$$

$$\Psi_3(t) = -0{\cdot}6593 + 0{\cdot}3420t + 0{\cdot}0276t^2 + 0{\cdot}0073t^3 + 0{\cdot}0026t^4 + 0{\cdot}0011t^5 + 0{\cdot}0004t^6 + 0{\cdot}0001t^7. \tag{2.12}$$

Only the leading amplitude is reasonably well defined and we estimate

$$A = 0{\cdot}963 \pm 0{\cdot}002. \tag{2.13}$$

## 3. Loose-packed lattices

For a loose-packed lattice the zeroth approximation

$$\beta_n = \mu \tag{3.1}$$

leads to an oscillatory sequence of estimates because of the presence of the antiferromagnetic singularity on the radius of convergence. The elementary treatment now supposes that near $T_C$

$$\chi \sim A(1-\mu v)^{-\gamma} + a(1+\mu v)^{-\alpha+1} \tag{3.2}$$

where the second term is introduced to represent the antiferromagnetic singularity. As already explained in I, the representation of the two singularities as a *sum* will be adequate asymptotically even if product terms are present. The antiferromagnetic critical behaviour is assumed to be the same as that of the *energy*; in other words $\alpha$ in (3.2) is assumed to be the critical index of the specific heat; the theoretical basis for this assumption is given in I.

The coefficients $a_n$ of the susceptibility expansion now follow from the binomial theorem; the contributions of the first and second term are asymptotically proportional to $n^{\gamma-1}\mu^n$ and $n^{\alpha-2}(-\mu)^n$ respectively. Thus if (3.2) were exact the ratios should contain an oscillation which declines asymptotically as $1/n^{\gamma-\alpha+1}$. In two dimensions $\alpha = 0$ and adopting $\gamma = 1{\cdot}75$ gives $1/n^{2\cdot75}$; we therefore expect the oscillation to fall off rapidly with $n$. In three dimensions $\alpha$ is not known exactly; adopting the hypothesis $\alpha = 0{\cdot}125$ (Sykes *et al* 1967, 1972b) and $\gamma = 1{\cdot}25$ we obtain $1/n^{2\cdot125}$; the oscillation should prove more persistent in three than in two dimensions.

Extending the analysis of § 2 we replace (3.2) by the more general assumption

$$\chi \sim (1-\mu v)^{-\gamma}\Phi_{\mathrm{f}}(v) + (1+\mu v)^{-\alpha+1}\Phi_{\mathrm{a}}(v) + \Psi(v) \tag{3.3}$$

where $\Phi_{\mathrm{f}}$, $\Phi_{\mathrm{a}}$ and $\Psi$ are regular in the disc $|v| \leqslant v_{\mathrm{f}}$. The corresponding asymptotic behaviour of $\beta_n$ is found to be

$$\beta_n = \mu\left(1 + \frac{\eta}{n^2} + \frac{\eta^*}{n^3} + \ldots + (-1)^n \frac{\zeta}{n^{\gamma-\alpha+1}} + (-1)^n \frac{\zeta^*}{n^{\gamma-\alpha+2}} + \ldots\right). \tag{3.4}$$

Despite the complexity introduced by the second singularity the conclusion that $\beta_n$ should become asymptotically linear against $1/n^2$ for large $n$ still holds. Following the general approach of the previous section the first order ferromagnetic approximation $\beta(1\text{F})$ is still

$$\beta_n = \mu\left(1 + \frac{\eta}{n^2}\right) \tag{3.5}$$

but we now solve for *alternate* pairs of $\beta_n$; the use of alternate pairs smooths out the even–odd oscillation. The first order antiferromagnetic approximation $\beta(1\text{A})$ we take as

$$\beta_n = \mu\left(1 + (-1)^n \frac{\zeta}{n^{\gamma-\alpha+1}}\right) \tag{3.6}$$

solved in the same way, although successive instead of alternate pairs of $\beta_n$ could be used in this case. Finally the combined first order approximation $\beta(1\text{F}, 1\text{A})$

$$\beta_n = \mu\left(1+\frac{\eta}{n^2}+(-1)^n\frac{\zeta}{n^{\gamma-\alpha+1}}\right) \tag{3.7}$$

is solved from successive triplets of $\beta_n$.

The estimates under these three approximations for the square lattice are illustrated in figure 3. For $\beta(1\text{F})$ there is a persistent even–odd effect but for $n > 12$ the values

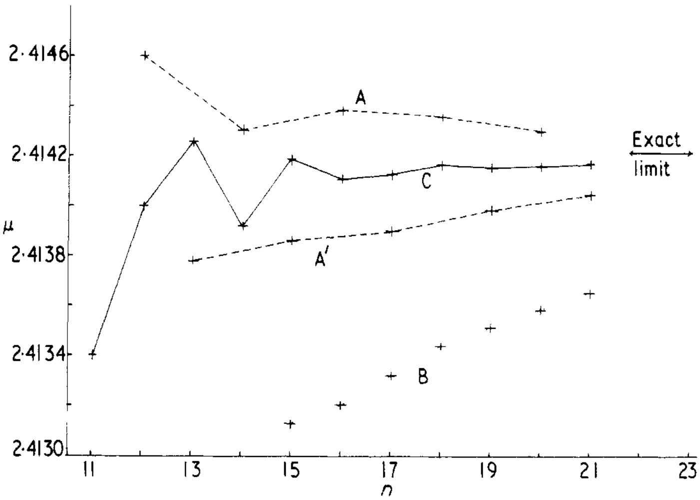


**Figure 3.** Square lattice. Estimates for $\mu = 1/v_c$. (A) First order ferromagnetic approximation $\beta(1\text{F})$. (B) First order antiferromagnetic approximation $\beta(1\text{A})$. (C) Combined first order approximation $\beta(1\text{F}, 1\text{A})$.

settle down to a fairly smooth behaviour; the last ten values are all within 1 part in 10 000 of the true limit. For $\beta(1\text{A})$ there is no detectable oscillation and a smooth behaviour again develops as $n$ increases; the approach to the true limit is slower because of the neglect of the nonoscillatory term in $1/n^2$. The combined approximation $\beta(1\text{F}, 1\text{A})$ takes account both of the quadratic term and the oscillation and gives a very good sequence of estimates for $\mu$ for $n > 15$; the last estimate is within 2 parts in 100 000. We have investigated higher approximations such as $\beta(2\text{F}, 1\text{A})$ by solving

$$\beta_n = \mu\left(1+\frac{\eta}{n^2}+\frac{\eta^*}{n^3}+(-1)^n\frac{\zeta}{n^{2\cdot75}}\right) \tag{3.8}$$

and found the number of coefficients available not adequate for these to provide any improvement.

The estimates under the same three approximations for the simple cubic lattice are illustrated in figure 4. The behaviour is similar to that of the square lattice. The antiferromagnetic approximation appears to converge more rapidly; this is partly because the index assumed for the oscillation (2·125) is now very close to the index for the nonoscillatory term, and partly because $\eta/\zeta$ for this lattice is of the order of 0·1. The fact that the oscillation is effectively smoothed for $\beta(1\text{A})$ supports the assumption that the critical index for the specific heat is very close to $\frac{1}{8}$; the procedure is quite

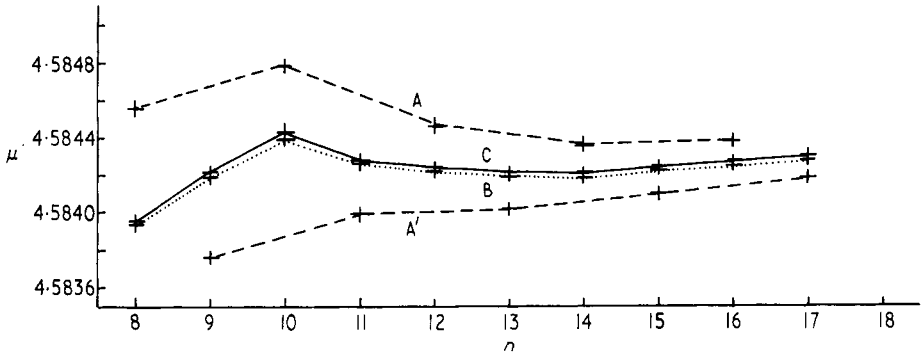


**Figure 4.** Simple cubic lattice. Estimates for $\mu = 1/v_c$. (A) First order ferromagnetic approximation $\beta(1\text{F})$. (B) First order antiferromagnetic approximation $\beta(1\text{A})$. (C) Combined first order approximation $\beta(1\text{F}, 1\text{A})$.

sensitive to small changes in this index. We estimate from the figure that

$$\mu = \frac{1}{v_f} = 4{\cdot}5844 \pm 0{\cdot}0002. \tag{3.9}$$

In making this estimate we have followed the indicated trend; in other words we have assumed that the limit $\mu$ is approached from *below* as it apparently is in two dimensions.

In a similar manner, and making the same assumptions, we estimate for the body-centred cubic lattice that

$$\mu = \frac{1}{v_f} = 6{\cdot}4055 \pm 0{\cdot}0010. \tag{3.10}$$

In this instance the steepness of approach seems slightly greater. We give the solutions to (3.7) for the square, simple cubic and body-centred cubic lattices in table 1.

We conclude from the data of table 1 that our assumptions are adequate and no more complicated form is required. Accordingly we generalize (2.8) and write

$$\chi \sim A(1-\mu v)^{-\gamma} + B(1-\mu v)^{-\gamma+1} + \ldots + a(1+\mu v)^{-\alpha+1} + b(1+\mu v)^{-\alpha+2} + \ldots + \Psi(v) \tag{3.11}$$

with $A, B, C, \ldots a, b, c, \ldots$ constants. In particular

$$\eta = \frac{-(\gamma-1)B}{A} \tag{3.12}$$

$$\zeta = \frac{2a\Gamma(\gamma)}{A\Gamma(\alpha-1)} \tag{3.13}$$

where in two dimensions $\Gamma(-1)$ is to be taken as unity. For the square lattice the values $A = 0{\cdot}7717$, $B = 0{\cdot}2003$ and $a = 0{\cdot}2003$ found in I yield $\eta = -0{\cdot}3374$ and $\zeta = -0{\cdot}4770$. The entries in table 1 are in reasonable agreement; the estimates of I are of course based on the known critical point.

The equations (3.12) and (3.13) cannot be exploited without first estimating the value of $A$. We have therefore re-analysed the series for the simple cubic and body-centred cubic lattices by fitting to the form (3.11) using the same procedure as in I with

**Table 1.** Solutions of $\beta_n = \mu\{1+\eta/n^2+(-1)^n\zeta/n^{\gamma-\alpha+1}\}$ assuming $\gamma = 1{\cdot}75$, $\alpha = 0$ in two dimensions and $\gamma = 1{\cdot}25$, $\alpha = 0{\cdot}125$ in three dimensions

| Triad | | | Square | | | Simple cubic | | | Body-centred cubic | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | $\eta$ | $\zeta$ | $\mu$ | $\eta$ | $\zeta$ | $\mu$ | $\eta$ | $\zeta$ | $\mu$ |
| 1 | 2 | 3 | −0·3047 | −0·2358 | 2·45491 | −0·0493 | −0·0930 | 4·59917 | −0·0878 | −0·0759 | 6·47711 |
| 2 | 3 | 4 | −0·0749 | −0·4133 | 2·37194 | −0·0354 | −0·0991 | 4·58936 | −0·0081 | −0·1112 | 6·39840 |
| 3 | 4 | 5 | −0·2854 | −0·5519 | 2·41161 | −0·0645 | −0·1084 | 4·60004 | −0·0248 | −0·1165 | 6·40692 |
| 4 | 5 | 6 | −0·2921 | −0·5473 | 2·41239 | −0·0208 | −0·1314 | 4·58098 | −0·0024 | −0·1226 | 6·39993 |
| 5 | 6 | 7 | −0.3659 | −0·5934 | 2·41823 | −0·0116 | −0·1334 | 4·58236 | −0·0285 | −0·1283 | 6·40539 |
| 6 | 7 | 8 | −0·2908 | −0·6409 | 2·41397 | −0·0032 | −0·1306 | 4·58395 | −0·0176 | −0·1304 | 6·40375 |
| 7 | 8 | 9 | −0·2302 | −0·6053 | 2·41138 | −0·0065 | −0·1311 | 4·58422 | −0·0271 | −0·1320 | 6·40483 |
| 8 | 9 | 10 | −0·3483 | −0·5356 | 2·41531 | −0·0098 | −0·1306 | 4·58443 | −0·0226 | −0·1327 | 6·40444 |
| 9 | 10 | 11 | −0·2770 | −0·4957 | 2·41341 | −0·0069 | −0·1302 | 4·58428 | −0·0270 | −0·1333 | 6·40474 |
| 10 | 11 | 12 | −0·3042 | −0·4805 | 2·41400 | −0·0058 | −0·1303 | 4·58423 | −0·0266 | −0·1333 | 6·40472 |
| 11 | 12 | 13 | −0·3186 | −0·4882 | 2·41426 | −0·0051 | −0·1302 | 4·58421 | −0·0301 | −0·1337 | 6·40489 |
| 12 | 13 | 14 | −0·2958 | −0·5004 | 2·41391 | −0·0055 | −0·1302 | 4·58422 | −0·0312 | −0·1336 | 6·40494 |
| 13 | 14 | 15 | −0·3171 | −0·5114 | 2·41419 | −0·0076 | −0·1304 | 4·58427 | −0·0343 | −0·1339 | 6·40504 |
| 14 | 15 | 16 | −0·3097 | −0·5151 | 2·41411 | −0·0074 | −0·1303 | 4·58426 | | | |
| 15 | 16 | 17 | −0·3117 | −0·5161 | 2·41413 | −0·0089 | −0·1305 | 4·58429 | | | |
| 16 | 17 | 18 | −0·3161 | −0·5140 | 2·41417 | | | | | | |
| 17 | 18 | 19 | −0·3146 | −0·5132 | 2·41416 | | | | | | |
| 18 | 19 | 20 | −0·3158 | −0·5126 | 2·41416 | | | | | | |
| 19 | 20 | 21 | −0·3177 | −0·5135 | 2·41418 | | | | | | |

the critical points (3.9) and (3.10) respectively. We have found that three parameters can be fitted and give the estimates for $A_2$, $B_2$ and $a_1$ in table 2. The ferromagnetic amplitudes ($A_2$) are reasonably well defined; the antiferromagnetic amplitudes ($a_1$) are increasing slowly. By graphical extrapolation we estimate

$$A = 1{\cdot}1016 \pm 0{\cdot}0010(\text{SC}) \qquad A = 0{\cdot}967 \pm 0{\cdot}003(\text{BCC}). \tag{3.14}$$

The values found by Fisher and Sykes (1962), using much shorter series, were 1·018 and 0·973 respectively; their critical temperatures were 0·01 % and 0·03 % lower respectively. The rather large discrepancy in the amplitude for the body-centred cubic lattice is probably accounted for by the relatively high value of $\eta$ or $B/A$ for this lattice which implies a slower convergence.

It is difficult to extrapolate the estimates for $a$ precisely but they seem consistent with the limits

$$a \simeq 0{\cdot}630(\text{SC}) \qquad a \simeq 0{\cdot}622(\text{BCC}) \tag{3.15}$$

calculated from (3.13) and (3.14) using

$$\zeta \simeq -0{\cdot}131(\text{SC}) \qquad \zeta \simeq -0{\cdot}135(\text{BCC}) \tag{3.16}$$

estimated from table 1. For the square lattice the estimate $\zeta \simeq -0{\cdot}514$ corresponds to an antiferromagnetic amplitude of 0·216 in reasonable agreement with the estimate $a \simeq 0{\cdot}22$ of I.

Using the independent estimates for the energy of Sykes *et al* (1972b) we calculate the corresponding values for the energetic approximation

$$a^{\mathrm{E}} \simeq 0{\cdot}604(\text{SC}) \qquad a^{\mathrm{E}} \simeq 0{\cdot}582(\text{BCC}). \tag{3.17}$$

**Table 2.** Estimates for the parameters $A_2, B_2, a_1$ assuming $\gamma = 1{\cdot}25$, $\alpha = 0{\cdot}125$

| Simple cubic $\mu = 4{\cdot}5844$ | | | | Body-centred cubic $\mu = 6{\cdot}4055$ | | | |
|---|---|---|---|---|---|---|---|
| $n$ | $A_2$ | $B_2$ | $a_1$ | $n$ | $A_2$ | $B_2$ | $a_1$ |
| 8 | 1·0164 | 0·0417 | 0·4848 | 8 | 0·9672 | 0·1274 | 0·4689 |
| 9 | 1·0167 | 0·0301 | 0·4996 | 9 | 0·9675 | 0·1210 | 0·4771 |
| 10 | 1·0164 | 0·0405 | 0·5135 | 10 | 0·9669 | 0·1430 | 0·5064 |
| 11 | 1·0166 | 0·0345 | 0·5218 | 11 | 0·9668 | 0·1444 | 0·5044 |
| 12 | 1·0164 | 0·0443 | 0·5358 | 12 | 0·9664 | 0·1613 | 0·5282 |
| 13 | 1·0164 | 0·0429 | 0·5378 | 13 | 0·9664 | 0·1651 | 0·5226 |
| 14 | 1·0162 | 0·0518 | 0·5510 | 14 | 0·9661 | 0·1784 | 0·5422 |
| 15 | 1·0162 | 0·0519 | 0·5509 | 15 | 0·9660 | 0·1826 | 0·5359 |
| 16 | 1·0161 | 0·0587 | 0·5613 | | | | |
| 17 | 1·0161 | 0·0590 | 0·5610 | | | | |

We conclude that, although the antiferromagnetic amplitude is difficult to determine with precision, the overall picture is reasonably consistent and parallels that in two dimensions; the amplitude is not very sensitive to lattice structure and differs at most by only a few percent from that indicated by the energetic approximation.

Following the method of I (§ 3) we represent the susceptibility by adopting the last entries in table 2 and allow for the departure of the earlier coefficients by a correction polynomial. Writing $t = v/v_{\mathrm{f}}$ we obtain for the simple cubic lattice (correct to 4 decimal places)

$$\begin{aligned}\chi(v) &\simeq 1{\cdot}0164(1-t)^{-1{\cdot}25}+0{\cdot}0472(1-t)^{-0{\cdot}25}\\ &\quad +0{\cdot}5622(1+t)^{0{\cdot}875}+\Psi_{2,1}(t)\\ \Psi_{2,1} &= -0{\cdot}6360-0{\cdot}4669t+0{\cdot}0200t^2-0{\cdot}0095t^3\\ &\quad -0{\cdot}0006t^4-0{\cdot}0021t^5-0{\cdot}0004t^6-0{\cdot}0009t^7\\ &\quad -0{\cdot}0003t^8-0{\cdot}0004t^9-0{\cdot}0001t^{10}-0{\cdot}0002t^{11}\end{aligned} \tag{3.18}$$

and for the body-centred cubic lattice

$$\begin{aligned}\chi(v) &\simeq 0{\cdot}9669(1-t)^{-1{\cdot}25}+0{\cdot}1581(1-t)^{-0{\cdot}25}\\ &\quad +0{\cdot}5388(1+t)^{0{\cdot}875}+\Psi_{2,1}(t)\\ \Psi_{2,1} &= -0{\cdot}6846-0{\cdot}4732t-0{\cdot}0072t^2-0{\cdot}0125t^3\\ &\quad -0{\cdot}0023t^4-0{\cdot}0037t^5-0{\cdot}0013t^6-0{\cdot}0014t^7\\ &\quad -0{\cdot}0006t^8-0{\cdot}0005t^9-0{\cdot}0002t^{10}-0{\cdot}0001t^{11}.\end{aligned} \tag{3.19}$$

Setting $t = -1$ we obtain estimates for the critical susceptibility of the antiferromagnet of

$$\chi_{\mathrm{a}} = 0{\cdot}3394(\textsc{sc}) \qquad \chi_{\mathrm{a}} = 0{\cdot}3693(\textsc{bcc}) \tag{3.20}$$

in very good agreement with the estimates of Fisher and Sykes (1962) of 0·3397 and 0·3692 respectively.

The evaluation of the critical susceptibility depends essentially on the summation of an alternating series; in these circumstances the remainder to be estimated is relatively small and not very sensitive to the representation adopted. This accounts for the close agreement with earlier estimates; (3.18) and (3.19) should represent the susceptibility numerically in the region of $T > T_C$ with an accuracy sufficient for most practical purposes. More complicated representations are required if the extrapolated amplitudes (3.15) are to be used; the numerical effect on the antiferromagnetic susceptibility is almost negligible.

## 4. Conclusion

We have compared the general pattern of asymptotic behaviour of susceptibility coefficients in two and three dimensions. We have found a very close resemblance; the data are consistent with the assumption that the values of certain critical parameters change with dimension, but not the functional form. For all three dimensional lattices the successive estimates for $1/v_f$ are increasing, although only slightly; the trend increases with coordination number and is most marked for the face-centred cubic lattice. It is implicit in the ratio method that we assume the indicated trends persist; they certainly appear to persist in two dimensions where the exact limit is known. On this basis we have made the estimates

$$\begin{aligned} &\text{SC} && \mu = 4{\cdot}5844 \pm 0{\cdot}0002 \\ &\text{BCC} && \mu = 6{\cdot}4055 \pm 0{\cdot}0010 \\ &\text{FCC} && \mu = 9{\cdot}8290 \pm 0{\cdot}0005. \end{aligned} \tag{4.1}$$

These may be compared with previous estimates, quoted by Fisher (1967), who gives an extensive bibliography, of

$$\begin{aligned} &\text{SC} && \mu = 4{\cdot}5840 \\ &\text{BCC} && \mu = 6{\cdot}4032 \\ &\text{FCC} && \mu = 9{\cdot}828. \end{aligned} \tag{4.2}$$

The changes are very small, being greatest for the body-centred cubic lattice and even then only 4 parts in 10 000. The new values are all higher on the temperature scale for the reasons stated; in particular we have assumed that the limits are approached in the same manner as they are in two dimensions. It is possible to argue that this is erroneous; such a criticism would carry more weight if based on evidence from an alternative source. Unfortunately no estimates other than those based on susceptibility expansions have so far achieved comparable precision.

The available data are consistent with the hypothesis that the susceptibility above the critical point is well represented by

$$\chi \sim (1-\mu v)^{-1{\cdot}25}\Phi_f(v) + (1+\mu v)^{0{\cdot}875}\Phi_a(v) + \Psi(v) \tag{4.3}$$

where $\Phi_f$, $\Phi_a$, and $\Psi$ are regular in the disc $|v| \leqslant v_f$. The estimation of the amplitudes $A = \Phi_f(v_f)$ and $a = \Phi_a(-v_f)$ is difficult because $v_f$ is not known exactly. The ferromagnetic amplitude is reasonably well defined; the amplitude of the much weaker antiferromagnetic singularity much less so. Final estimates, consistent with (4.1) are

$$\begin{aligned} A &= 1{\cdot}0163 \pm 0{\cdot}0010(\text{SC}) = 0{\cdot}9667 \pm 0{\cdot}003(\text{BCC}) \\ &= 0{\cdot}963 \pm 0{\cdot}002(\text{FCC}) \end{aligned} \tag{4.4}$$

and near $v = v_f$ the ferromagnetic susceptibility behaves approximately as

$$\chi \sim A_T(1 - T_C/T)^{-1\cdot 25} \qquad T \to T_C+ \tag{4.5}$$

with

$$A_T = 1\cdot 0585 \pm 0\cdot 0010(\text{SC}) = 0\cdot 9868 \pm 0\cdot 003(\text{BCC}) = 0\cdot 971 \pm 0\cdot 002(\text{FCC}). \tag{4.6}$$

Near $v = -v_f$ the antiferromagnetic susceptibility behaves approximately as

$$\left.\begin{aligned} \chi &\simeq 0\cdot 3394 + 0\cdot 630(1 + v/v_f)^{0\cdot 875} & v &\to v_a + \\ &\phantom{\simeq}\ 0\cdot 3394 + 0\cdot 612(1 - T_N/T)^{0\cdot 875} & T &\to T_N + \end{aligned}\right\} (\text{SC}) \tag{4.7}$$

$$\left.\begin{aligned} \chi &\simeq 0\cdot 3692 + 0\cdot 622(1 + v/v_f)^{0\cdot 875} & v &\to v_a + \\ &\phantom{\simeq}\ 0\cdot 3692 + 0\cdot 613(1 - T_N/T)^{0\cdot 875} & T &\to T_N + \end{aligned}\right\} (\text{BCC}) \tag{4.8}$$

where the amplitudes are within a few percent of independent estimates of the energetic approximation.

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**Appendix**

Expansions for the reduced zero-field susceptibility in powers of the high temperature counting variable $v = \tanh K$ (equation (1.1)).

Simple cubic lattice:

$$\begin{aligned} \chi = {} & 1 + 6v + 30v^2 + 150v^3 + 726v^4 + 3510v^5 + 16710v^6 + 79494v^7 \\ & + 375174v^8 + 1769686v^9 + 8306862v^{10} + 38975286v^{11} \\ & + 182265822v^{12} + 852063558v^{13} + 3973784886v^{14} \\ & + 18527532310v^{15} + 86228667894v^{16} + 401225391222v^{17} \ldots \end{aligned}$$

Body-centred cubic lattice:

$$\begin{aligned} \chi = {} & 1 + 8v + 56v^2 + 392v^3 + 2648v^4 + 17864v^5 + 118760v^6 + 789032v^7 \\ & + 5201048v^8 + 34268104v^9 + 224679864v^{10} + 1472595144v^{11} \\ & + 9619740648v^{12} + 62823141192v^{13} + 409297617672v^{14} \\ & + 2665987056200v^{15} \ldots \end{aligned}$$

Face-centred cubic lattice:

$$\begin{aligned} \chi = {} & 1 + 12v + 132v^2 + 1404v^3 + 14652v^4 + 151116v^5 + 1546332v^6 \\ & + 15734460v^7 + 159425580v^8 + 1609987708v^9 + 16215457188v^{10} \\ & + 162961837500v^{11} + 1634743178420v^{12} \ldots \end{aligned}$$

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