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LETTER TO THE EDITOR

# High-temperature reduced susceptibility of the Ising model

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**Abstract.** Two new coefficients are given for the high-temperature series expansion of the zero-field susceptibility of the Ising model for the face-centred cubic lattice. The new coefficients are analysed and it is estimated that the critical temperature $v_c = \tanh K_c = 0{\cdot}10173 \pm 0{\cdot}00001$ and the critical index $\gamma = 1{\cdot}250 \pm 0{\cdot}005$.

The use of exact series expansions in the study of the three-dimensional Ising model is well known. A comprehensive review is given by Domb (1973). High-temperature series expansions have been extensively used for the determination of critical points and critical exponents. In particular, the exponent ($\gamma$) associated with the high-temperature zero-field susceptibility ($\chi_0$) is of relevance in the study of thermodynamic scaling (Brout 1973 and references cited therein). The asymptotic behaviour of the coefficients in the $\chi_0$ series has been discussed by Sykes *et al* (1972). We have extended the series by two terms and show that the new terms are consistent with their proposed asymptotic form within narrow limits. On this basis we make a slightly more precise estimate for the critical temperature.

Several methods have been used in the past to derive the high-temperature reduced susceptibility series. The most successful have been the counting theorem approach (Sykes 1961), the renormalized linked cluster expansion (Moore *et al* 1969) and the finite cluster series development (Domb and Hiley 1962). The first was used to extend the susceptibility series on the face-centred cubic (FCC) lattice to 12 terms (Sykes *et al* 1972). The linked cluster expansion is more general in nature and gives the spin–spin correlation functions, but has been used to calculate the 12th term in the $\chi_0$ series for the FCC lattice, though incorrectly (Moore *et al* 1969).

The cluster series development has only recently been exploited for this problem. It was first described by Yvon (1945) who applied the Mayer cluster integral technique to the discrete lattice and showed how a series of successive closed approximations could be obtained. A similar approach due to Fuchs (1942) was developed by Rushbrooke and Scoins (1955) for binary mixed crystals. Rushbrooke and Scoins showed that despite multiple occupation of the lattice points, nonzero contributions to the cluster sums can only arise from those configurations in which the lattice sites are multiply connected. Domb and Hiley (1962) extended the method of Yvon to a wide variety of lattice problems, including the Ising zero-field susceptibility. They used the Mayer theory for multi-component systems and showed how the reduced susceptibility $\chi_0$ for a cluster $G$ could be expressed in the form

$$\chi_0^{-1}(v) = \sum_S (S\,; G) W_S(v) \tag{1}$$

where the sum is over all star subgraphs $S$ of $G$, $(S; G)$ is the weak lattice constant of $S$ on $G$ and $W_S(v)$ is a 'weights' polynomial in the usual high-temperature counting variable $v$ (= tanh $J/kT$), associated with $S$ but independent of $G$. Generalization to an infinite lattice presents no difficulty.

This method was used by Rapaport (1974) to calculate the 13th term in the high-temperature $\chi_0$ series for the FCC lattice. We present here the next two terms in the series obtained by the same method. The list of contributing star graphs which was already extensive at the 13th order becomes even more so at the 15th. Over 30 000 star graphs were considered and rather specialized data handling techniques had to be developed. Considerable care was taken to ensure that all contributions were included, and it is hoped that no significant errors remain.

On performing the summation in (1) for $S \leqslant 15$ and inverting we find:

$$\begin{aligned}\chi_0 = {} & 1+12v+132v^2+1\,404v^3+14\,652v^4+151\,116v^5+1\,546\,332v^6+15\,734\,460v^7 \\ & +159\,425\,580v^8+1\,609\,987\,708v^9+16\,215\,457\,188v^{10} \\ & +162\,961\,837\,500v^{11}+1\,634\,743\,178\,420v^{12} \\ & +16\,373\,484\,437\,340v^{13}+163\,778\,159\,931\,180v^{14} \\ & +1\,636\,328\,839\,130\,860v^{15}+\dots\end{aligned}$$

The terms to 13th order are in agreement with previous calculations (Sykes *et al* 1972, Rapaport 1974).

Neville table estimates for $v_c^{-1}$ are given in table 1. From these we make the estimate that

$$v_c^{-1} = 9{\cdot}8300 \pm 0{\cdot}0005. \qquad (2)$$

**Table 1.** Neville table estimates for $v_c^{-1}$.

| | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| 9 | 10·09868 | 9·83006 | 9·82802 | 9·82442 |
| 10 | 10·07179 | 9·82979 | 9·82870 | 9·83028 |
| 11 | 10·04978 | 9·82973 | 9·82946 | 9·83149 |
| 12 | 10·03145 | 9·82975 | 9·82989 | 9·83119 |
| 13 | 10·01594 | 9·82980 | 9·83008 | 9·83073 |
| 14 | 10·00265 | 9·82986 | 9·83018 | 9·83051 |
| 15 | 9·99113 | 9·82991 | 9·83024 | 9·83052 |

This is very slightly higher than the estimate of Sykes *et al* (1972) of

$$v_c^{-1} = 9{\cdot}8295 \pm 0{\cdot}0005. \qquad (3)$$

The Neville table estimates for the critical exponent ($\gamma$) for $v_c^{-1} = 9{\cdot}830$ are given in table 2. From these we make the estimate that

$$\gamma = 1{\cdot}246 \pm 0{\cdot}005. \qquad (4)$$

Though the value is somewhat lower than 1·25, it is not in serious conflict with the view that $\gamma$ tends to $\frac{5}{4}$, when one considers the inaccuracies inherent in any extrapolation procedure.

**Table 2.** Neville table estimates for $\gamma$.

| | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| 9 | 1·24599 | 1·24604 | 1·24463 | 1·24122 |
| 10 | 1·24597 | 1·24578 | 1·24471 | 1·24491 |
| 11 | 1·24594 | 1·24566 | 1·24517 | 1·24638 |
| 12 | 1·24592 | 1·24564 | 1·24553 | 1·24662 |
| 13 | 1·24590 | 1·24566 | 1·24575 | 1·24650 |
| 14 | 1·24588 | 1·24569 | 1·24591 | 1·24648 |
| 15 | 1·24587 | 1·24574 | 1·24607 | 1·24670 |

Following Sykes *et al* (1972), we have made 'biased' estimates of $v_c^{-1}$, based on the assumption that $\gamma$ is exactly $\frac{5}{4}$. We have solved the first- and second-order approximations to the formula:

$$\beta_n = v_c^{-1}\left(1+\frac{\xi}{n^2}+\frac{\xi^*}{n^3}+\frac{\xi^{**}}{n^4}+\ldots\right)$$

where $\beta_n = na_n/a_{n-1}(n+\gamma-1)$ with $a_n$ = coefficient of $v^n$ in the $\chi_0$ series. The results are illustrated in figure 1.

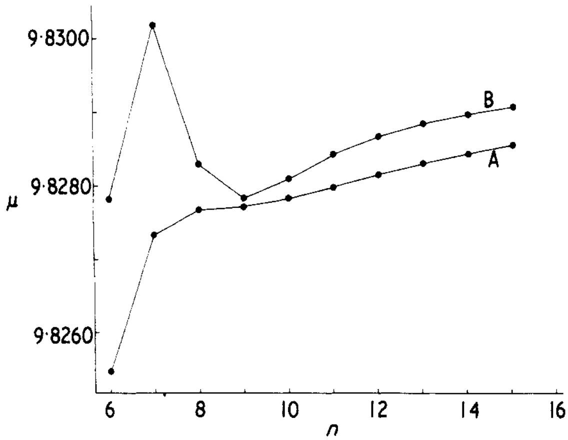


**Figure 1.** Estimates for $\mu = v_c^{-1}$. A, first-order approximation: B, second-order approximation.

The new points fall very smoothly into place, confirming the asymptotic behaviour proposed by Sykes *et al* (1972). However, there is still an upward trend justifying a slight revision of the critical point; a graphical extrapolation of the last five points against $1/n$ is in agreement with (2).

We conclude therefore that the new terms in the susceptibility series confirm the proposed asymptotic form within very narrow limits, though leading to a slight revision of the critical point. Added support is lent to the hypothesis that $\gamma$ is exactly $\frac{5}{4}$ in three dimensions. Details of the derivation of the new coefficients will be published in due course.

The list of star-graph lattice constants for the face-centred cubic lattice was compiled as part of the research programme of the Theoretical Physics Group of King's College. I am most grateful to my colleagues Dr M F Sykes, Dr D S McKenzie and Dr M G Watts for their assistance in its compilation and for their advice at all stages of this project. I am also particularly indebted to Professor C Domb and Dr B J Hiley for much constructive advice on the theory of the star-graph expansion for susceptibilities.

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