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Extended high-temperature series for the classical Heisenberg model in three dimensions

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Abstract. Extended series expansions are derived for the high-temperature susceptibility of the classical Heisenberg model, on three-dimensional lattices. Series coefficients are presented to twelfth order for the simple cubic (SC) and face centred cubic (FCC) lattices and to eleventh order for the body centred cubic (BCC) lattice. Our results are in agreement with earlier calculations apart from a small discrepancy at the tenth order on the FCC lattice. In addition, this work extends earlier series by two terms on the FCC and SC lattices and by one term on the BCC lattice. Extrapolation studies on the extended series are used to obtain revised estimates for the critical points (K_c) and the susceptibility exponent (γ). On the FCC lattice, we also investigate the possibility of a confluent non-analytic correction to the dominant singularity. While the coefficients are consistent with the presence of such a correction term with an exponent (Δ_1) of 0.55, as predicted by renormalisation group (RG) calculations, the amplitude of the correction term appears to be very small compared with that of the first analytic correction term. Our estimate for γ is in excellent agreement with RG predictions, but is somewhat lower than those of Ferer *et al* and Camp and Van Dyke.

1. Introduction

We investigate the zero field susceptibility of the three-dimensional classical Heisenberg model above the critical temperature. The model has been widely studied (see for instance, Rushbrooke *et al* 1974), and is characterised by the Hamiltonian

$$\mathscr{H} = -J\sum_{\langle ij\rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - mH\sum_{i=1}^{N} \sigma_i^z. \tag{1}$$

The $\boldsymbol{\sigma}_i$ ($i = 1, 2, 3, \ldots N$) are three-dimensional classical unit vectors representing magnetic spins on the N sites of a three-dimensional lattice. The first sum is over all nearest-neighbour pairs of spins, where J denotes the interaction energy between such pairs. An external magnetic field H is assumed to act in the z direction. The

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magnetic moment of a spin is denoted by m and σ_i^z is the z component of $\boldsymbol{\sigma}_i$. From (1), the partition function Z_N, free energy F_N and the zero field susceptibility χ_0 are defined in the usual manner:

$$Z_N = \mathrm{Tr}\exp(-\mathcal{H}/kT), \qquad F_N = -kT\ln Z, \qquad \chi_0 = \frac{kT}{N}\frac{\partial^2 \ln Z_N}{\partial H^2}\bigg|_{H=0}. \tag{2}$$

Various methods have been used in deriving series expansions for the Heisenberg model. These include the moment and cumulant methods (Rushbrooke and Wood 1958, Stanley 1967), the finite cluster development (Joyce and Bowers 1966) and the linked cluster expansion (Ferer *et al* 1971). More recently, the star graph expansion method has been used to extend the zero field free energy series on the FCC lattice (English *et al* 1979). The existence of a star graph expansion for the inverse susceptibility (χ_0^{-1}) of the Ising and classical n-vector models was shown by Domb (1972, 1976). The method has been used mainly for the Ising model (McKenzie 1975, 1980a,b). In this paper we generalise the procedure to the classical Heisenberg model ($n=3$) and derive extended series for the zero field susceptibility on the three-dimensional lattices. A brief discussion of the derivation together with the new series coefficients is given in § 2. We quote two new terms for the FCC and simple cubic lattices and one new term for the BCC lattice.

Earlier extrapolation studies on susceptibility series were based on the assumption of a dominant power law singularity modified by analytic correction terms. Thus

$$\chi_0 \sim A(t)t^{-\gamma}, \qquad t = 1 - T_c/T. \tag{3}$$

The amplitude $A(t)$, being a slowly varying function of t, gives rise to weaker correction terms of the Darboux type (Gaunt and Guttmann 1974). Estimates for γ based on this assumption range from $1.375 \pm ^{0.02}_{0.01}$ (Ritchie and Fisher 1972) to 1.405 ± 0.02 (Ferer *et al* 1971). Recent RG calculations, however, predict the existence of a non-analytic correction term modifying the singularity (3). This term is characterised by a correction-to-scaling exponent Δ_1, which has the value 0.55 (Baker *et al* 1978, Le Guillou and Zinn-Justin 1977). Studies by Camp and Van Dyke (1976) explicitly incorporate this correction term into the analysis and result in the estimates $\gamma = 1.42 \pm ^{0.02}_{0.01}$, $\Delta_1 = 0.54 \pm 0.10$ for the classical Heisenberg model. While their estimate for Δ_1 is certainly consistent with RG calculations, that for γ is significantly higher than the RG predictions of 1.39 ± 0.01 (Baker *et al* 1978) and 1.3866 ± 0.0012 (Le Guillou and Zinn-Justin 1977).

In § 3, we analyse the extended susceptibility series by standard extrapolation methods to obtain revised estimates for the critical temperatures and the exponent γ for the three lattices. Analysing for the asymptotic form (3), without including the non-analytic term, we find that $\gamma = 1.39 \pm 0.01$ for all three lattices. This is in excellent agreement with RG predictions and with earlier series estimates excepting those of Ferer *et al* (1971) and Camp and Van Dyke. We then proceed to incorporate the correction-to-scaling term by using the method of four-parameter fits (Camp and Van Dyke 1975, 1976). This latter analysis has been confined to the FCC lattice as the loose packed lattices present difficulties owing to the antiferromagnetic singularity (Camp and Van Dyke 1975). We find that while it is possible to fit the series coefficients using a correction-to-scaling term with an exponent of 0.55, the amplitude of this term is extremely small compared with that of the first analytic correction. The value of the dominant exponent 'γ' remains practically unchanged.

2. Derivation of series

Following Domb (1976) and McKenzie (1980b), we develop the inverse susceptibility (χ_1^{-1}) as a star graph expansion. For a lattice, we write

$$\chi_0^{-1}(\mathscr{L}) = \sum_S (S;\mathscr{L}) h_s(\omega), \tag{4}$$

where the sum is over all star graphs S which can be embedded on the lattice. $(S;\mathscr{L})$ denotes the weak lattice constant of S on $\mathscr{L}$ defined per site. $h_s(\omega)$ is the weight or contribution of S to the susceptibility expansion and is a function of the variable ω defined by

$$\omega(K) = I_{3/2}(K)/I_{1/2}(K). \tag{5}$$

$I_l(K)$ denotes the modified Bessel function of the first kind, with $K = J/kT$. For purposes of deriving series expansions, the $h_s(\omega)$ can be developed as power series in K and truncated at the required order n. The sum in (4) is then restricted to star graphs with up to n edges and the expansion for χ_0^{-1} is correct to order K^n.

The weights $h_s(\omega)$ are calculated recursively by applying (4) in slightly modified form to finite star graphs. For a finite graph with N vertices, we can write

$$3kT\chi_N/m^2 = N + 2\sum_{i>j} \langle \sigma_i^z \sigma_j^z \rangle_{H=0}, \tag{6}$$

where the sum is over all pairs of vertices, and $\langle \sigma_i^z \sigma_j^z \rangle_{H=0}$ represents the correlation between the z components of spins i and j in zero field. As shown in Domb (1972), these correlation terms can be very simply related to the zero field partition function Z_0 of the graph S_{ij}^* constructed from S by joining vertices i and j by a pseudo edge with interaction K^*. Thus

$$\langle \sigma_i^z \sigma_j^z \rangle_{H=0} = \frac{1}{3} \left. \frac{\partial \ln Z_0(S_{ij}^*)}{\partial K^*} \right|_{K^*=0}. \tag{7}$$

The zero field partition function Z_0 is calculated using the procedures described in Domb (1976) as developed by English *et al* (1979). Having calculated χ_N for a star graph S, one can apply (4) to calculate $h_s(\omega)$ if the weights of all the star subgraphs are known. In this case, (4) takes the form

$$\chi_N^{-1}(S) = \sum_{S' \leqslant S} (S';S) h_{s'}(\omega). \tag{8}$$

The sum is now over all star subgraphs S' of S and $(S';S)$ denotes the total number of weak embeddings of S' on S. By considering star graphs in the order of increasing cycle index, one ensures that at any stage all the weights $h_s(\omega)$ have already been calculated except for $S' = S$, which is obtained from (8).

A slightly different procedure has to be adopted for inhomogeneous graphs. The reasons for this are discussed in detail in Domb and Hiley (1962) in the context of the Ising model and McKenzie (1980b) for the n-vector model. The left-hand side of (8) cannot be calculated by taking the reciprocal of (6). To get the correct results for an inhomogeneous graph, it is necessary to invert the matrix $\boldsymbol{M}$ of pair correlations defined as follows:

$$M_{ij} = \langle \sigma_i^z \sigma_j^z \rangle, \qquad M_{ii} = 1. \tag{9}$$

The LHS of (8) is now given by

$$\mathbf{1}^{\mathrm{T}}\boldsymbol{M}^{-1}\mathbf{1}=\mathbf{1}^{\mathrm{T}}(\boldsymbol{I}+\boldsymbol{X})^{-1}\mathbf{1}=\mathbf{1}^{\mathrm{T}}(\boldsymbol{I}-\boldsymbol{X})(\boldsymbol{I}+\boldsymbol{X}^2)(\boldsymbol{I}+\boldsymbol{X}^4)\ldots\mathbf{1}. \tag{10}$$

Expanding $\boldsymbol{M}^{-1}$ to the required order is sufficient for purposes of obtaining a series expansion and is much less time consuming than the usual methods of matrix inversion.

By considering all star graphs S with up to n edges, in the order of increasing cycle index, use of (7)–(10) yields the weights $h_s(\omega)$ which, together with the lattice constants for the appropriate lattice, yield $\chi_0^{-1}(K)$ through (4). It is then straightforward to derive $\chi_0(K)$ to the same order in K. We thus obtain

$$\begin{aligned}
&\text{SC:}\quad 3\chi_0=1+2K+3.3\dot{3}K^2+\ldots 158.232\,4883K^{11}+235.759\,9086K^{12}\\
&\text{BCC:}\quad 3\chi_0=1+2.66\dot{6}K+6.22\dot{2}K^2+\ldots 6878.945\,964K^{11}+\ldots\\
&\text{FCC:}\quad 3\chi_0=1+4K+14.66\dot{6}K^2+\ldots 246\,802.5993K^{10}+810\,503.9650K^{11}\\
&\qquad\qquad +2\,654\,798.191K^{12}+\ldots.
\end{aligned} \tag{11}$$

The coefficients on the SC and BCC lattices are in agreement with earlier calculations (Rushbrooke *et al* 1974) to tenth order. The remaining terms are new. On the FCC lattice, the coefficients to K^9 are in agreement with Ferer *et al* (1971). There is a very small discrepancy (in the eighth significant figure) at the next order. The coefficients of K^{11} and K^{12} are new.

We have incorporated various checks in our calculations to reduce the possibility of errors. The lattice constants have been used for a variety of other problems where series have been obtained by more than one method. We have also derived rules relating the weights of star graphs to those of higher cycle index (McKenzie 1976). These rules are independent of the scheme developed above. All these checks reveal no discrepancies and we trust that nothing of significance has been overlooked.

3. Extrapolation studies on the extended series

We first analyse for the dominant singularity (3) using Padé approximants and ratio methods (Gaunt and Guttmann 1974).

Estimates for the critical point (K_c) and the exponent γ are obtained from the roots and residues of successive Padé approximants to the logarithmic derivatives of the susceptibility series for the three lattices. A sample of estimates for the SC lattice is given in table 1 and the 'best' estimates for all three lattices are quoted in table 4.

Neville table sequences μ_n^m for K_c^{-1} are constructed from the ratios $R_n(=a_n/a_{n-1})$ of successive coefficients of the susceptibility series, using

$$\mu_n^m=[n\mu_n^{m-1}-(n-m)\mu_{n-1}^{m-1}]/m, \qquad \mu_n^0=R_n. \tag{12}$$

Sequences for γ_n^m are calculated in the same way, with

$$\gamma_n^0=1+n(R_n/\mu_n^1-1). \tag{13}$$

Thus the estimates for γ are unbiased by any arbitrary choice of K_c (Gaunt and Sykes 1979).

For the loose packed lattices (SC and BCC), we reduce the interference from the antiferromagnetic singularity by transforming to a variable x, given by

$$x=2K/(1+K/K_c). \tag{14}$$

Table 1. SC lattice, Padé approximants to the logarithmic derivative. Roots (K_c) and residues (γ).

$D \backslash N$	3	4	5	6	7	8
3		0.692 70 1.391	0.692 73 1.392	0.692 19 1.384	0.692 49 1.390	0.692 27 1.386
4	0.684 11 1.303	0.691 89 1.380	0.692 25 1.385	0.692 30 1.386	0.691 81 1.381	
5	0.692 00 1.382	0.692 59 1.391	0.692 32 1.387	0.692 21 1.385		
6	0.692 35 1.387	0.692 34 1.387	0.692 45 1.389			
7	0.692 34 1.387	0.692 34 1.387				
8	0.691 99 1.382					

The transformation has the effect of removing the antiferromagnetic singularity ($K = -K_c$) to infinity, leaving the ferromagnetic ($K = K_c$) singularity unaltered. Neville table sequences formed from the transformed series do not show the characteristic odd–even oscillation (Gaunt and Guttmann 1974) and yield smooth estimates for x_c and γ. A preliminary estimate for K_c is required to perform the transformation. This is obtained from the Padé approximants. Having made a final estimate of x_c, we recover the value of K_c by using (14). Tables of sequences for the FCC (untransformed series) and the SC (transformed series) lattices are presented in tables 2 and 3 while the 'best' estimates for all three lattices are given in table 4.

Table 2. FCC lattice, Neville tables of sequences of K_c^{-1} and γ.

	K_c^{-1}				γ	
$n \backslash m$	0	1	2	3	0	1
6	3.365 66					
7	3.340 65	3.190 61			1.329	
8	3.321 54	3.187 70	3.178 98		1.336	1.383
9	3.306 42	3.185 47	3.177 65	3.174 99	1.342	1.388
10	3.294 16	3.183 82	3.177 24	3.176 27	1.347	1.390
11	3.284 02	3.182 61	3.177 15	3.176 93	1.350	1.390
12	3.275 49	3.181 70	3.177 15	3.177 14	1.354	1.389

Table 3. SC lattice, susceptibility series in the variable $x = 2K/(1+K/K_c)$, with $K_c^{-1} = 1.4443$. Neville table sequences for x_c^{-1} and γ.

	x_c^{-1}			γ	
$n \backslash m$	0	1	2	0	1
7	1.506 02	1.464 46		1.199	
8	1.500 27	1.460 02	1.446 69	1.221	1.374
9	1.495 43	1.456 72	1.445 20	1.239	1.388
10	1.491 31	1.454 28	1.444 51	1.255	1.394
11	1.487 78	1.452 46	1.444 28	1.267	1.396
12	1.484 72	1.451 09	1.444 24	1.278	1.395

Table 4. Estimates for K_c and γ from ratio analysis and Padé approximants.

	Padé approximants		Ratio method	
Lattice	K_c	γ	K_c	γ
SC	0.6924 ± 0.0002	1.387 ± 0.004	0.6925 ± 0.0001	1.395 ± 0.005
BCC	0.4868 ± 0.0003	1.390 ± 0.005	0.4868 ± 0.0004	1.393 ± 0.005
FCC	0.3147 ± 0.0002	1.381 ± 0.01	0.3148 ± 0.0001	1.390 ± 0.005

On the basis of this analysis, we conclude that $\gamma = 1.39 \pm 0.01$ is a reasonable estimate for all three lattices. This is in agreement with most earlier series estimates (Ritchie and Fisher 1972 and references cited therein) and with RG predictions (Baker *et al* 1978, Le Guillou and Zinn–Justin 1977). It is, however, significantly lower than the value of $1.42^{+0.02}_{-0.01}$ obtained by Camp and Van Dyke (1976) after incorporating a non-analytic correction-to-scaling term.

To investigate the presence of such correction terms, we consider a more general asymptotic form in place of (3). We assume

$$\begin{aligned}\chi_0 &= A(K)(1-K/K_c)^{-\gamma} + B(K)(1-K/K_c)^{-\gamma+\Delta_1}\\ &= A_1(1-K/K_c)^{-\gamma} + B_1(1-K/K_c)^{-\gamma+\Delta_1} + A_2(1-K/K_c)^{-\gamma+1}.\end{aligned} \tag{15}$$

The term involving $A(K)$ is the dominant term as in (3), and gives rise to a series of Darboux-type analytic terms which diverge as γ, $\gamma-1$ and so on. The term involving $B(K)$ represents the correction-to-scaling term, with exponent Δ_1. Expanding $B(K)$ in Taylor series results in a series of correction terms with amplitudes B_1, B_2 and so on. We truncate the sequences A_n and B_n at A_2 and B_1 respectively so as to keep the number of parameters to be fitted to a manageable level.

The method of four fits (Camp and Van Dyke 1975, 1976, Camp *et al* 1976) was used to estimate the correction-to-scaling exponent Δ_1 and the other parameters in (15). Three variants of the method were used and the results are presented in tables 5 to 7. The details of the method are discussed below. The analysis was confined to the FCC lattice for reasons discussed in § 1.

From (15), it can be shown that the ratios $R_n (= a_n/a_{n-1})$, in the limit of large n, behave as

$$R_n \approx K_c^{-1}\left(1 + \frac{\gamma-1}{n} + \frac{a}{n^{1+\Delta_1}} + \frac{b}{n^2}\right). \tag{16}$$

The amplitudes a and b are simply related to B_2/A_1 and A_2/A_1 (Camp and Van Dyke 1975). For fixed choices of γ and Δ_1, we solve successive triplets R_n, 1_{n-1}, R_{n-2} for a, b and K_c^{-1}. As can be seen from table 5, best converged sequences are obtained for $\gamma = 1.387 \pm 0.003$, $\Delta_1 = 0.55$. We make the estimates

$$K_c^{-1} = 3.1771 \pm 0.0002, \qquad \gamma = 1.387 \pm 0.003, \qquad a = 0.00 \pm 0.01,$$
$$b = -0.19 \pm 0.02. \tag{17}$$

The amplitude 'a' of the correction-to-scaling term is extremely small, suggesting that the first analytic correction term is the more important of the two.

We next adopt a free fit procedure for Δ_1. Neglecting the b/n^2 term in (16), we use successive triplets of R_n to solve for a, γ and Δ_1 for fixed choices of K_c. The

Table 5. FCC lattice. Sequences for K_c^{-1}, a and b obtained by solving (16) for various choices of γ with Δ_1 set to 0.55.

	$\gamma = 1.38$			$\gamma = 1.39$		
n	K_c^{-1}	a	b	K_c^{-1}	a	b
7	3.180 05	−0.041	−0.087	3.179 12	−0.078	−0.052
8	3.178 82	−0.009	−0.145	3.178 02	−0.050	−0.103
9	3.177 96	0.019	−0.198	3.177 26	−0.025	−0.150
10	3.177 65	0.032	−0.223	3.177 03	−0.016	−0.168
11	3.177 55	0.036	−0.232	3.176 99	−0.014	−0.172
12	3.177 52	0.038	−0.237	3.177 01	−0.015	−0.170

	$\gamma = 1.387$			$\gamma = 1.40$		
n	K_c^{-1}	a	b	K_c^{-1}	a	b
7	3.179 40	−0.067	−0.062	3.178 19	−0.116	−0.016
8	3.178 26	−0.037	−0.116	3.177 22	−0.091	−0.061
9	3.177 47	−0.012	−0.164	3.176 56	−0.069	−0.102
10	3.177 22	−0.002	−0.185	3.176 41	−0.063	−0.114
11	3.177 16	0.001	−0.190	3.176 43	−0.065	−0.111
12	3.177 16	0.001	−0.190	3.176 50	−0.068	−0.104

Table 6. FCC lattice. Sequences for γ, Δ_1 and a obtained by solving (16) for various choices of K_c^{-1} with $b = 0$.

		$K_c^{-1} = 3.175$				$K_c^{-1} = 3.178$	
n	γ	Δ_1	a	n	γ	Δ_1	a
8	1.436	0.434	−0.165	8	1.388	0.822	−0.145
9	1.423	0.540	−0.164	9	1.381	1.082	−0.186
10	1.423	0.534	−0.164	10	1.379	1.231	−0.225
11	1.430	0.474	−0.162	11	1.378	1.327	−0.259
12	1.440	0.398	−0.161	12	1.377	1.412	−0.297

		$K_c^{-1} = 3.177$	
n	γ	Δ_1	a
8	1.400	0.671	−0.145
9	1.392	0.863	−0.166
10	1.389	0.937	−0.179
11	1.389	0.951	−0.182
12	1.389	0.942	−0.180

results for three different choices of K_c are shown in table 6. We make the estimate

$$\gamma = 1.388 \pm 0.002, \qquad \Delta_1 = 0.98 \pm 0.04, \qquad a = -0.18 \pm 0.005,$$
$$K_c^{-1} = 3.1771 \pm 0.0001. \tag{18}$$

The fact that Δ_1 is so close to 1 confirms our earlier suggestion that the $1/n^2$ term dominates the $1/n^{1+\Delta_1}$ term in (16).

Both the fitting procedures discussed above involve the R_n through (16), which is derived using certain approximations which are true only when n is very large. To eliminate any errors due to this approximation, we also carry out a third procedure,

Table 7. FCC lattice. Sequences of γ, Δ_1, A_1 and B_1 obtained by solving (15) with A_2 set to zero, for various choices of K_c^{-1}.

		$K_c^{-1}=3.176$					$K_c^{-1}=3.1774$		
n	γ	Δ_1	A_1	B_1	n	γ	Δ_1	A_1	B_1
8	1.415	0.570	0.726	0.273	8	1.396	0.692	0.785	0.233
9	1.406	0.675	0.763	0.261	9	1.388	0.863	0.814	0.266
10	1.404	0.699	0.769	0.262	10	1.386	0.951	0.823	0.313
11	1.406	0.675	0.764	0.260	11	1.385	0.993	0.826	0.347
12	1.408	0.634	0.754	0.257	12	1.384	1.017	0.828	0.373

		$K_c^{-1}=3.177$		
n	γ	Δ_1	A_1	B_1
8	1.401	0.653	0.770	0.241
9	1.393	0.803	0.802	0.256
10	1.390	0.868	0.810	0.279
11	1.390	0.885	0.812	0.288
12	1.390	0.884	0.812	0.287

where the series coefficients (a_n) are used directly to solve for A_1, B_1, γ and Δ_1 for various choices of K_c, with A_2 in (15) set to zero. Again, the free fit for Δ_1 should pick out the dominant correction term whether it be analytic or non-analytic. The results, shown in table 7, lead to the estimates

$$K_c^{-1}=3.1771\pm0.0001, \qquad \gamma=1.388\pm0.002, \qquad \Delta_1=0.91\pm0.03,$$
$$A_1=0.815\pm0.005, \qquad B_1=0.300\pm0.010. \tag{19}$$

Again Δ_1 is extremely close to 1, confirming the estimate from our previous analysis.

4. Conclusions

Extended series expansions are derived for the high-temperature, zero field susceptibility of the classical Heisenberg model in three dimensions. The star graph expansion method is used and the derivation of series is discussed. New coefficients are presented for three lattices.

The extended series are analysed by standard extrapolation techniques and revised estimates are presented for the critical point (K_c) and the susceptibility exponent γ. The estimate $\gamma=1.39\pm0.01$ seems to be a reasonable choice for all three lattices, and is in good agreement with RG calculations and most earlier series estimates.

The method of four fits is used to investigate the presence of non-analytic correction terms predicted by RG calculations. We find that while a fit is possible with the predicted correction-to-scaling exponent Δ_1 of 0.55, the amplitude of this term is extremely small compared with that of the first analytic correction. The values of K_c and γ remain practically unchanged.

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