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COMMENT

The high-temperature susceptibility of the classical Heisenberg model in four dimensions

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Abstract. The high-temperature susceptibility of the four-dimensional classical Heisenberg model is studied by the method of series expansions. High-temperature series are presented to order K^9 for the hyper face centred (HFCC) lattice, to order K^{11} for the hyper body centred cubic (HBCC) lattice and to order K^{12} for the hyper simple cubic (HSC) lattice. The last three coefficients for the HSC lattice and all the coefficients for the other two lattices are new. The series are analysed for singularities of the form $t^{-1}|\ln t|^p$, predicted by the renormalisation group theory ($t = 1 - K_c/K$, where K is the high-temperature expansion variable J/kT). Fairly good convergence is obtained for $p \approx 0.45$ for all three lattices, in agreement with renormalisation group calculations.

In a previous paper (McKenzie *et al* 1982, hereafter referred to as I), we investigated the high-temperature susceptibility of the classical Heisenberg model in three dimensions. The star graph expansion method was used to derive extended series expansions on several three-dimensional lattices. In this paper, we extend the calculations to four-dimensional lattices and derive series expansions for the HFCC, HBCC and HSC lattices. The series are analysed by various extrapolation methods and the results are presented.

As discussed in I, the star graph expansion for the susceptibility takes the form

$$\chi_0^{-1}(\mathcal{L}) = \sum_{S \leq \mathcal{L}} (S; \mathcal{L}) h_s(\omega) = \sum_{n=0} a_n K^n \quad (1)$$

where \mathcal{L} denotes the lattice; the sum is over all star graphs S which can be embedded on \mathcal{L} , with weak lattice constant $(S; \mathcal{L})$. The $h_s(\omega)$ represent the weights or contributions of the star graphs S to the reciprocal susceptibility expansion and are functions of the variable ω given by

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

The $I_l(K)$ denote modified Bessel functions of the first kind, and K is the usual high-temperature variable J/kT . The calculation of $h_s(\omega)$ as power series in ω (and hence of K) is discussed in I. The weights $h_s(\omega)$ depend only on the star graph S and

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not on the lattice \mathcal{L} . Thus the same set of $h_s(\omega)$ can be used, together with the appropriate $(S; \mathcal{L})$, to obtain susceptibility series for any lattice. We have done this for the four-dimensional analogues HFCC, HBCC and HSC of the corresponding three-dimensional lattices, FCC, BCC and SC. The lattice constants were obtained using standard methods (see for instance, Martin 1974), together with some special techniques for the low index graphs (Sykes *et al* 1972). Use of (1) then yields the following series for χ_0 :

$$\begin{aligned}
 \text{HFCC: } & 1 + 8K + 61.333K^2 + 460.8K^3 + 3427.081\,4814K^4 + 25\,336.586\,596K^5 \\
 & + 186\,584.132\,06K^6 + 1370\,266.8804K^7 + 10\,042\,618.427K^8 \\
 & + 73\,485\,823.889K^9 + \dots \\
 \text{HBCC: } & 1 + 5.33\dot{3}K + 26.66\dot{6}K^2 + 132.97\dot{7}K^3 + 653.234\,567\,90K^4 \\
 & + 3205.301\,3521K^5 + 15\,633.457\,965K^6 + 76\,205.145\,397K^7 \\
 & + 370\,296.145\,78K^8 + 1798\,686.4767K^9 + 8720\,393.2376K^{10} \\
 & + 42\,267\,736.713K^{11} + \dots \\
 \text{HSC: } & 1 + 2.66\dot{6}K + 6.22\dot{2}K^2 + \dots + 4051.065\,4878K^{10} \\
 & + 8998.094\,1908^{11} + 19\,957.360\,710K^{12} + \dots
 \end{aligned} \tag{3}$$

The series coefficients for the HSC lattice are in agreement with Stanley (1974) to order K^9 . The last three coefficients for this lattice are new and so are all the coefficients for the HBCC and HFCC lattices. Various checking procedures used to ensure the correctness of the lattice constants and weights are described in I and they have been incorporated in these calculations as well.

The four-dimensional ($d = 4$) classical Heisenberg model has not been studied as extensively as its three-dimensional counterpart. Stanley (1974) investigates the more general classical n -vector[†] model on the d -dimensional hypercubical lattices and concludes that the critical properties are monotonic functions of the spin dimensionality n . Thus the properties of the classical Heisenberg model ($n = 3$) are bounded between those of the Ising model ($n = 1$) and those of the spherical model ($n = \infty$). On the basis of exact solutions ($n = \infty$, all d and $d = 1$, all n), as well as available series expansions on the hypercubical lattices, Stanley conjectured that the susceptibility exponent (γ) assumes the mean field value of 1 for all n if $d \geq 4$.

This conjecture finds support in renormalisation group (RG) calculations (Brézin *et al* 1976, for instance) which predict the existence of a logarithmic correction term modifying the simple power law singularity. Thus, the asymptotic behaviour of χ_0 for $d = 4$ (all n) is given by

$$\chi_0 \sim At^{-\gamma} |\ln t|^p \quad (\gamma = 1), \tag{4}$$

where $t = 1 - K/K_c$. p is the exponent of the logarithmic correction term and depends on the value of n . For $n = 3$ (the classical Heisenberg model), $p = \frac{5}{11}$.

To analyse the series (3) for the asymptotic form (4), we use a method due to Guttman (1978) which has been extensively applied to the $d = 4$ Ising model (McKenzie 1979, McKenzie *et al* 1979, Gaunt *et al* 1979, McKenzie and Gaunt

[†] Stanley used the letter D to represent spin dimension but in recent years the letter n (following Wilson) has received wider acceptance.

1980). The method consists in comparing the coefficients a_n of the susceptibility series (3) with those of the mimic function $f(K)$ defined by

$$f(K) = K^{-p^*}(1-K)^{-1} [\ln[1/(1-K)]]^{p^*} = \sum b_n K^n. \quad (5)$$

We form the ratios

$$R_n = (a_n/a_{n-1})/(b_n/b_{n-1}), \quad (6)$$

which should approach K_c^{-1} with zero slope as $n \rightarrow \infty$ for $p^* = p$.

A slightly modified procedure is necessary for the loose packed lattices to eliminate interference from the antiferromagnetic singularity (Guttmann 1978). We first transform (3) to a new variable x given by

$$x = 2K/(1 + K/K_c), \quad (7)$$

and use the coefficients of the transformed series in place of the a_n in (6). A preliminary estimate of K_c is required for the transformation (7) and this is obtained by forming Padé approximants to the logarithmic derivative of the series (3).

In tables 1–3 we present sequences of Padé approximants for the critical point (K_c) and the exponent (γ) for the three lattices. We include the HFCC for completeness, though the transformation (7) is, strictly speaking, not necessary in this case. On the basis of these sequences, we make the following estimates for the critical points K_c :

$$K_c = \begin{cases} 0.456\,15 \pm 0.0002 & (\text{HSC}), \\ 0.2083 \pm 0.0003 & (\text{HBCC}), \\ 0.138\,38 \pm 0.000\,05 & (\text{HFCC}). \end{cases} \quad (8)$$

The estimates for γ are higher than the mean field value of 1, but that may be due either to slow convergence of the series or to the fact that the logarithmic correction term has not been included in the analysis.

We now analyse for the logarithmic exponent p using the procedure outlined above. We compute the sequences R_n defined in (6), using the transformation (7), with K_c given by (8). For the correct choice of p^* , the R_n should tend to x_c^{-1} for

Table 1. HSC lattice. Estimates for K_c and γ from Padé approximants to the logarithmic derivative of the susceptibility series.

D/N	3	4	5	6	7	8
3	0.456 21 (1.137)	0.455 94 (1.134)	0.455 92 (1.134)	0.455 70 (1.129)	0.455 85 (1.132)	0.455 49 (1.124)
4	0.455 93 (1.134)	0.455 80 (1.131)	0.456 18 (1.135)	0.456 16 (1.135)	0.458 12 (1.058)	
5	0.455 84 (1.132)	0.456 12 (1.135)	0.456 16 (1.135)	0.456 18 (1.135)		
6	0.456 27 (1.135)	0.456 16 (1.135)	0.456 12 (1.135)			
7	0.456 16 (1.135)	0.456 25 (1.135)				
8	0.457 36 (1.104)					

Table 2. HBCC lattice. Estimates for K_c and γ from Padé approximants to the logarithmic derivative of the susceptibility series.

D/N	3	4	5	6	7
3	0.208 37 (1.105)	0.208 35 (1.104)	0.208 35 (1.104)	0.208 27 (1.101)	0.208 29 (1.102)
4	0.208 35 (1.104)	0.208 38 (1.105)	0.209 74 [†] (0.900 4)	0.208 04 (1.081)	
5	0.208 39 (1.105)	0.208 08 (1.085)	0.208 08 (1.086)		
6	0.207 12 [†] (0.881)	0.208 08 (1.086)			
7	0.208 06 (1.083)				

[†] Defective approximants.**Table 3.** HFCC lattice. Estimates for K_c and γ from Padé approximants to the logarithmic derivative of the susceptibility series.

N/D	2	3	4	5	6
2	0.140 12 (1.074)	0.138 41 (1.114)	0.138 38 (1.113)	0.138 39 (1.113)	0.138 33 (1.108)
3	0.138 42 (1.115)	0.138 38 (1.113)	0.138 38 (1.113)	0.138 38 (1.113)	
4	0.138 39 (1.113)	0.138 38 (1.113)	0.138 38 (1.113)		
5	0.138 38 (1.113)	0.138 39 (1.113)			
6	0.138 38 (1.113)				

$n \rightarrow \infty$. To allow for higher-order correction terms, linear and quadratic extrapolants of R_n are calculated. Simultaneously, the 'exponent' estimates $n(R_n x_c - 1)$ and their linear extrapolants must approach zero as $n \rightarrow \infty$. The sequences for R_n and their linear and quadratic extrapolants together with sequences for the exponent and linear extrapolants are presented in tables 4–6 for the three lattices.

In all three cases, the R_n and their extrapolants tend to a value of K_c^{-1} reasonably consistent with the Padé estimates (8). However, the convergence is not sufficiently rapid for us to decide on the best choice of p^* from these sequences alone. A better criterion, which also has the advantage of not being biased by the initial choice of K_c^{-1} , is that of requiring that the sequence of 'exponents' and that of their linear extrapolants must vanish for the correct choice of p^* . We find that for the HSC lattice, the exponents are all positive for $p^* = 0.4$, becoming extremely small and negative for $p^* = 0.4545$ and increasing in magnitude (while still negative) for $p^* = 0.5$. This suggests that they will tend to zero for some value of p^* close to, possibly a little less

Table 4. HSC lattice. Analysis for the logarithmic exponent.

p^*	n	R_n	Linear extrapolants	Quadratic extrapolants	Exponent	Linear extrapolants
0.4	7	2.1885	2.2105	2.1973	-0.0121	0.0377
	8	2.1908	2.2069	2.1963	-0.0055	0.0413
	9	2.1923	2.2044	2.1957	+0.0001	0.0441
	10	2.1934	2.2026	2.1953	0.0048	0.0472
	11	2.1941	2.2013	2.1951	0.0089	0.0497
	12	2.1946	2.2002	2.1950	0.0125	0.0522
0.454 545	7	2.1829	2.2117	2.1981	-0.0300	0.0231
	8	2.1861	2.2080	2.1969	-0.0228	0.0273
	9	2.1882	2.2054	2.1962	-0.0168	0.0309
	10	2.1897	2.2034	2.1957	-0.0117	0.0340
	11	2.1908	2.2020	2.1954	-0.0073	0.0369
	12	2.1917	2.2009	2.1953	-0.0034	0.0396
0.5	7	2.1782	2.2127	2.1987	-0.0449	0.0109
	8	2.1821	2.2089	2.1974	-0.0374	0.0156
	9	2.1847	2.2061	2.1966	-0.0310	0.0195
	10	2.1867	2.2041	2.1961	-0.0256	0.0239
	11	2.1881	2.2026	2.1957	-0.0209	0.0261
	12	2.1892	2.2014	2.1955	-0.0168	0.0290

Table 5. HBCC lattice. Analysis for the logarithmic exponent.

p^*	n	R_n	Linear extrapolants	Quadratic extrapolants	Exponent	Linear extrapolants
0.4	6	4.7608	4.8476	4.8143	-0.0490	0.0005
	7	4.7716	4.8368	4.8098	-0.0414	0.0046
	8	4.7789	4.8294	4.8073	-0.0352	0.0076
	9	4.7839	4.8242	4.8059	-0.0302	0.0101
	10	4.7875	4.8204	4.8052	-0.0260	0.0123
	11	4.7903	4.8175	4.8047	-0.0223	0.0142
0.454 545	6	4.7461	4.8505	4.8165	-0.0673	-0.0147
	7	4.7594	4.8394	4.8114	-0.0591	-0.0099
	8	4.7685	4.8317	4.8086	-0.0525	-0.0063
	9	4.7749	4.8262	4.8070	-0.0471	-0.0034
	10	4.7796	4.8222	4.8060	-0.0425	-0.0009
	11	4.7832	4.8191	4.8054	-0.0385	+0.0014
0.5	6	4.7339	4.8529	4.8185	-0.0827	-0.0276
	7	4.7492	4.8415	4.8129	-0.0740	-0.0222
	8	4.7598	4.8335	4.8098	-0.0670	-0.0181
	9	4.7673	4.8278	4.8079	-0.0612	-0.0148
	10	4.7730	4.8236	4.8068	-0.0563	-0.0120
	11	4.7773	4.8204	4.8061	-0.0520	-0.0094

than, the predicted value of $\frac{5}{11}$. For the other two lattices, the sequences of linear extrapolants of the exponents behave in the same way. Thus, $p^* = \frac{5}{11}$ seems to be a reasonable choice for all three lattices, given the shortness of the series and the uncertainties in the extrapolation procedure.

Table 6. HFCC lattice. Analysis for the logarithmic exponent.

p^*	n	R_n	Linear extrapolants	Quadratic extrapolants	Exponent	Linear extrapolants
0.4	5	7.1940	7.2687	7.2523	-0.0225	-0.0009
	6	7.2052	7.2613	7.2465	-0.0177	-0.0064
	7	7.2124	7.2560	7.2428	-0.0136	-0.0109
	8	7.2174	7.2519	7.2397	-0.0101	-0.0145
	9	7.2209	7.2489	7.2383	-0.0070	-0.0178
0.454 545	5	7.1664	7.2743	7.2568	-0.0416	-0.0151
	6	7.1830	7.2661	7.2496	-0.0361	-0.0087
	7	7.1940	7.2601	7.2452	-0.0315	-0.0036
	8	7.2017	7.2555	7.2416	-0.0274	+0.0006
	9	7.2073	7.2520	7.2398	-0.0239	0.0043
0.5	5	7.1434	7.2786	7.2606	-0.0575	-0.0286
	6	7.1645	7.2699	7.2524	-0.0515	-0.0215
	7	7.1786	7.2634	7.2473	-0.0464	-0.0157
	8	7.1886	7.2584	7.2432	-0.0420	-0.0111
	9	7.1959	7.2545	7.2411	-0.0381	-0.0071

We conclude therefore that the high-temperature susceptibility of the four-dimensional classical Heisenberg model behaves consistently with RG predictions. The exponent of the logarithmic correction term is close to the predicted value of $\frac{5}{11}$.

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