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Susceptibility and fourth-field derivative of the spin-$\frac{1}{2}$ Ising model for $T > T_c$ and $d = 4$

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Abstract. We investigate the spin-$\frac{1}{2}$ Ising model with nearest-neighbour interactions on the four-dimensional simple hypercubic lattice. High-temperature series expansions are studied for the zero-field susceptibility χ_0 and the fourth-field derivative of the free energy $\chi_0^{(2)}$ up to order v^{17}. The series are analysed for singularities of the form $t^{-q}|\ln t|^p$ where t is the reduced temperature. For χ_0 it is found that $p = 0{\cdot}33 \pm 0{\cdot}07$ when $q = 1$, in good agreement with the prediction $p = \frac{1}{3}$, $q = 1$ of renormalisation group theory. The critical temperature is estimated to be $v_c^{-1} = 6{\cdot}7315 \pm 0{\cdot}0015$. Results for $\chi_0^{(2)}$ are more slowly convergent but are not inconsistent with the renormalisation group prediction $p = \frac{1}{3}$, $q = 4$.

1. Introduction and summary

An early study of the spin-$\frac{1}{2}$ Ising model with nearest-neighbour interactions on lattices with more than three space-like dimensions is that of Fisher and Gaunt (1964). They obtained the high-temperature expansion for the zero-field susceptibility χ_0 on a general simple hypercubic lattice of dimensionality d in the usual high-temperature variable $v = \tanh (J/kT)$ up to order v^{11}. At that time it was generally believed that as $T \to T_c+$

$$\chi_0 \sim t^{-\gamma} \qquad t = (T - T_c)/T_c \tag{1.1}$$

where the critical exponent γ approaches its mean-field value of $\gamma = 1$ smoothly as $d \to \infty$. Support for this conjecture was obtained by Fisher and Gaunt by analysing their series using the standard ratio and Padé approximant techniques, which have been reviewed by Gaunt and Guttmann (1974). However, according to the modern theory of the renormalisation group (for reviews of RG, see Fisher 1974, Ma 1976, Brézin *et al* 1976, Wallace and Zia 1978) γ is expected to decrease from $\gamma = 1\frac{3}{4}$ when $d = 2$, attain its mean-field value of $\gamma = 1$ at the critical dimension ($d_c = 4$) and then remain at this value for all $d > 4$. Fisher and Gaunt, however, estimated that in four dimensions

$$\gamma = 1{\cdot}094 \pm 0{\cdot}0025 \qquad (d = 4). \tag{1.2}$$

Larkin and Khmel'nitskii (1969) showed by the use of field-theoretical techniques that the asymptotic form of the susceptibility for $d = 4$ should include a logarithmic correction term in addition to the $t^{-\gamma}$ dependence. They predicted that, in contrast to

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(1.1), χ_0 should behave as

$$\chi_0 \sim t^{-\gamma}|\ln t|^p, \qquad (T \to T_c+) \tag{1.3}$$

with $\gamma = 1$ and $p = \frac{1}{3}$.

The first attempt to explain discrepancies like that between (1.2) and the mean-field value $\gamma = 1$ in terms of a confluent logarithmic singularity was made by Moore (1970). He concluded that his series expansions for the spherical moments of the spin–spin correlation function were suggestive of logarithmic factors, but was unable to distinguish between them and a real departure of the indices from their mean-field values. Assuming the asymptotic form (1.1), he estimated $\gamma = 1{\cdot}065 \pm 0{\cdot}003$, a value slightly smaller than (1.2) of Fisher and Gaunt.

Recently, Baker (1977) has derived a high-temperature expansion up to order v^9 for the fourth-field derivative of the free energy $\chi_0^{(2)}$ on a simple hypercubic lattice of arbitrary dimensionality. Using this series together with the susceptibility expansion and a revised estimate of the exponent ν for the correlation length ξ he obtained for $d = 4$

$$2\Delta - d\nu - \gamma = -0{\cdot}302 \pm 0{\cdot}038 \tag{1.4}$$

where Δ is the gap exponent. This result is in direct conflict with RG theory which assumes implicitly that the hyperscaling relation

$$2\Delta - d\nu - \gamma = 0 \tag{1.5}$$

holds exactly in all dimensions. In four dimensions, RG theory predicts that algebraic singularities are modified by the presence of logarithmic correction terms. As we have seen, the susceptibility is given by (1.3) while the fourth-field derivative becomes (Brézin *et al* 1976)

$$\chi_0^{(2)} \sim t^{-\gamma-2\Delta}|\ln t|^p \qquad (T \to T_c+) \tag{1.6}$$

with $\gamma = 1$, $\Delta = \frac{3}{2}$ and $p = \frac{1}{3}$. Hence,

$$\chi_0^{(2)}/\chi_0 \sim t^{-3} \tag{1.7}$$

and should be free of logarithmic factors. By considering quantities such as $\chi_0^{(2)}/\chi_0$ and $\chi_0\xi^4$, both of which are logarithm-free according to RG theory, Baker (1977) concluded that the singularity structure of the high-temperature series for χ_0, $\chi_0^{(2)}$, $\xi, \ldots$ is more easily accounted for *without* the inclusion of logarithmic correction terms.

Clearly the failure of hyperscaling and the absence of logarithmic corrections for the four-dimensional Ising model would have important consequences for RG theory. In view of this we have undertaken an extensive study of the $d = 4$ Ising model. The basic configurational problem is studied in an accompanying paper (Sykes 1979) and the data derived there determine the expansions of χ_0 and $\chi_0^{(2)}$ up to v^{17}, namely

$$\begin{aligned}\chi_0 = {} & 1 + 8v + 56v^2 + 392v^3 + 2696v^4 + 18\,536v^5 + 126\,536v^6 \\ & + 863\,720v^7 + 5\,873\,768v^8 + 39\,942\,184v^9 + 271\,009\,112v^{10} \\ & + 1\,838\,725\,896v^{11} + 12\,457\,092\,504v^{12} + 84\,392\,312\,392v^{13} \\ & + 571\,140\,732\,808v^{14} + 3\,865\,210\,690\,888v^{15} \\ & + 26\,138\,072\,412\,040v^{16} + 176\,752\,645\,540\,264v^{17} + \ldots\end{aligned} \tag{1.8}$$

and

$$\chi_0^{(2)} = 1+32v+584v^2+8288v^3+101\,240v^4+1\,121\,120v^5 + 11\,570\,360v^6+113\,293\,088v^7+1\,064\,631\,032v^8 + 9\,681\,082\,144v^9+85\,688\,330\,696v^{10}+741\,562\,925\,664v^{11} + 6\,296\,196\,525\,768v^{12}+52\,589\,092\,312\,288v^{13} + 433\,044\,168\,426\,616v^{14}+3\,521\,747\,918\,221\,984v^{15} + 28\,326\,976\,016\,327\,032v^{16}+225\,625\,290\,121\,278\,496v^{17}+\ldots. \tag{1.9}$$

The χ_0 series are in agreement with Fisher and Gaunt (1964) up to v^{11}, while the $\chi_0^{(2)}$ series agrees with Baker (1977) up to v^9. All the other coefficients are new.

We have analysed these series for singularities of the form $t^{-q}|\ln t|^p$ using a method devised by Guttmann (1978) for dealing with a similar singularity in the generating function for self-avoiding walks on a four-dimensional simple hypercubic lattice. For χ_0 we estimate $p = 0{\cdot}33 \pm 0{\cdot}07$ when $q = 1$, while for $\chi_0^{(2)}$ $p = \frac{1}{3}$ provides a reasonably good fit to the data when $q = 4$. Both of these results are consistent with the predictions of RG theory, namely $q = 1$, $p = \frac{1}{3}$ for χ_0 and $q = 4$, $p = \frac{1}{3}$ for $\chi_0^{(2)}$.

Of course, by choosing values of q close to but not equal to their mean-field values it is possible to obtain an equally good fit to the data for slightly different values of p. Similarly, if one ignores the confluent logarithmic terms altogether by setting $p = 0$, a reasonably good fit can be obtained for values of q differing by relatively large amounts from their mean-field values. This explains why Fisher and Gaunt's original estimate (1.2) of γ was rather larger than the mean-field value. Reanalysis of the χ_0 series subject to this condition (namely $p = 0$) is undertaken in § 2 using the additional coefficients now available, mainly to provide an improved estimate of the critical point which we need for our subsequent analysis. We do not present our more general attempts to fit the series with fixed q not equal to its mean-field value. While such fits will presumably always be possible, the relative ease with which we have obtained estimates of p consistent with RG theory when q is fixed at its mean-field value may well be significant.

2. Series analysis of χ_0

As already stated, we need an approximate starting value of the critical point v_c. Using the standard ratio method (Gaunt and Guttmann 1974) we have analysed the χ_0 series on the assumption of a singularity of the form (1.1) and obtained an 'unbiased' estimate of

$$1/v_c = 6{\cdot}732 \pm 0{\cdot}002. \tag{2.1}$$

This is somewhat larger than the previous estimates of $6{\cdot}7220 \pm 0{\cdot}0015$ (Fisher and Gaunt 1964) and 6·725 (Moore 1970), which were based upon six fewer terms.

A 'biased' sequence of estimates for the exponent γ may be obtained from $\gamma_n = 1 + n(v_c\mu_n - 1)$ where μ_n is the ratio of successive coefficients. Using the central value in (2.1) we find 1·0788, 1·0862, 1·0764, 1·0823, 1·0742, 1·0792, 1·0722 and 1·0764 for $n = 10$ to 17. The uncertainty in (2.1) produces an uncertainty of $\pm 0{\cdot}005$ in the values of γ_n. Clearly the estimate (1.2) of Fisher and Gaunt (1964) is too large. However, the above sequence exhibits quite a lot of curvature when plotted against $1/n$ and is very difficult to extrapolate. Such behaviour would not be unexpected if (1.1) were modified by a confluent logarithmic correction term as in (1.3). Since a limiting value of $\gamma = 1$ is by no means excluded, we now analyse the series for a singularity of the form (1.3) with $\gamma = 1$, as predicted by RG theory.

Our more sophisticated analysis follows Guttmann (1978). One begins by eliminating the effect of the antiferromagnetic singularity by transforming to a new variable x defined by

$$x = 2v/[1+(v/v_c^*)] \tag{2.2}$$

where v_c^* is an estimate of the exact critical point v_c. We have used the central value in (2.1) for v_c^*. Writing the transformed series as

$$\chi_0(x) = \sum_{n \geq 0} a_n x^n$$

we next calculate the ratios $r_n = a_n/a_{n-1}$. Defining the function $f(x)$ by

$$x^{-p^*} f(x) \equiv x^{-p^*}(1-x)^{-q^*} |\ln(1-x)|^{p^*} = \sum_{n \geq 0} b_n x^n \tag{2.3}$$

with $q^* = 1$, we calculate the ratios $r_n^* = b_n/b_{n-1}$. The basic idea of the method is now to compare the behaviour of the ratios r_n^* for the mimic function (2.3) for a range of the parameter p^* with the behaviour of r_n. Our analysis is based upon the following two observations. Firstly, as $n \to \infty$ the sequence $R_n = r_n/r_n^*$ should approach x_c^{-1} with zero slope when $p^* = p$. To allow for higher-order correction terms, linear and quadratic extrapolants are calculated. Secondly, and simultaneously, the exponent estimates $n(R_n v_c^* - 1)$ and their linear extrapolants must approach zero as $n \to \infty$.

We have computed the above quantities for a range of values of p^* (holding $1/v_c^*$ fixed) and our results for four different values are shown in table 1. For $p^* = 0{\cdot}25$ the sequence $\{R_n\}$ increases, reaches a maximum and then decreases towards $1/v_c^*$. The linear and quadratic extrapolants are decreasing and increasing, respectively, towards $1/v_c^*$. However, the exponent estimates are increasing and are already well above zero. For $p^* = 0{\cdot}30$, $\{R_n\}$ is increasing and is already greater than $1/v_c^*$. However, it appears that a maximum is just about to be attained since the linear and quadratic extrapolants are decreasing and increasing, respectively, towards $1/v_c^*$. The exponent estimates, although increasing beyond zero, have linear extrapolants moving towards and closer to zero than they were in the previous case. Thus $p^* = 0{\cdot}30$ is favoured over $p^* = 0{\cdot}25$. For $p^* = 0{\cdot}35$ the $\{R_n\}$ sequence is approaching $1/v_c^*$ from below and the quadratic extrapolants are closer to $1/v_c^*$ than before. In addition, the exponent estimates are increasing towards zero from below but their linear extrapolants, although very close indeed to zero, are now moving away. This value of p^* seems equally acceptable as the previous one. For $p^* = 0{\cdot}40$ the quadratic extrapolants are marginally closer to $1/v_c^*$ than they were for $p^* = 0{\cdot}35$. However, the linear extrapolants of the exponent estimates are appreciably negative and moving even further away from zero. Thus, $p^* = 0{\cdot}40$ is less favoured than $p^* = 0{\cdot}35$. From this analysis alone we conclude that $p = 0{\cdot}30$ to $0{\cdot}35$. Similar results are obtained using other values of $1/v_c^*$ lying within the uncertainty range quoted in (2.1). Allowing for all the uncertainties, we widen our

Table 1. Analysis of transformed susceptibility series for the $d = 4$ Ising model assuming $1/v_c^* = 6{\cdot}732$.

p^*	n	R_n	Linear extrapolants	Quadratic extrapolants	Exponent	Linear extrapolants
	9	6·7387	6·7491	6·7270	0·0090	0·0293
	10	6·7393	6·7447	6·7271	0·0109	0·0278
	11	6·7395	6·7415	6·7273	0·0123	0·0264
	12	6·7395	6·7392	6·7276	0·0133	0·0251
0·25	13	6·7393	6·7375	6·7280	0·0142	0·0239
	14	6·7391	6·7362	6·7284	0·0148	0·0228
	15	6·7388	6·7352	6·7287	0·0153	0·0219
	16	6·7386	6·7344	6·7290	0·0156	0·0210
	17	6·7383	6·7338	6·7293	0·0159	0·0202
	9	6·7274	6·7518	6·7282	−0·0062	0·0173
	10	6·7293	6·7470	6·7281	−0·0039	0·0162
	11	6·7306	6·7436	6·7282	−0·0022	0·0150
	12	6·7315	6·7411	6·7284	−0·0009	0·0139
0·30	13	6·7321	6·7392	6·7286	0·0002	0·0129
	14	6·7325	6·7377	6·7289	0·0010	0·0120
	15	6·7328	6·7366	6·7292	0·0017	0·0112
	16	6·7330	6·7357	6·7295	0·0023	0·0105
	17	6·7331	6·7350	6·7297	0·0027	0·0098
	9	6·7160	6·7544	6·7295	−0·0214	0·0052
	10	6·7193	6·7494	6·7291	−0·0189	0·0044
	11	6·7217	6·7457	6·7291	−0·0168	0·0035
	12	6·7235	6·7429	6·7292	−0·0152	0·0027
0·35	13	6·7248	6·7408	6·7293	−0·0139	0·0019
	14	6·7258	6·7392	6·7295	−0·0128	0·0011
	15	6·7266	6·7380	6·7298	−0·0119	0·0005
	16	6·7273	6·7370	6·7300	−0·0112	−0·0001
	17	6·7278	6·7362	6·7302	−0·0106	−0·0007
	9	6·7045	6·7571	6·7308	−0·0368	−0·0070
	10	6·7092	6·7517	6·7302	−0·0339	−0·0075
	11	6·7127	6·7478	6·7300	−0·0315	−0·0081
	12	6·7154	6·7448	6·7300	−0·0296	−0·0087
0·40	13	6·7175	6·7425	6·7300	−0·0281	−0·0093
	14	6·7191	6·7408	6·7302	−0·0268	−0·0099
	15	6·7205	6·7394	6·7303	−0·0257	−0·0104
	16	6·7216	6·7383	6·7305	−0·0247	−0·0108
	17	6·7225	6·7374	6·7306	−0·0239	−0·0112

confidence limits and write

$$p = 0{\cdot}33 \pm 0{\cdot}07. \qquad (2.4)$$

This result is in good agreement with the RG prediction of $p = \frac{1}{3}$.

We now assume that the RG prediction (1.3) with $\gamma = 1$ and $p = \frac{1}{3}$ is the exact asymptotic behaviour and use this information to obtain an improved, 'biased' estimate of $1/v_c$. We use an analysis technique similar to that just described except that instead of varying p^* with $1/v_c^*$ held fixed, we vary $1/v_c^*$ with fixed $p^* = \frac{1}{3}$. In this way we estimate

$$1/v_c = 6{\cdot}7315 \pm 0{\cdot}0015 \qquad (2.5)$$

which lies very close to our initial 'unbiased' estimate in (2.1).

3. Series analysis of $\chi_0^{(2)}$

In this section we study the expansion (1.9) of the fourth-field derivative of the free energy $\chi_0^{(2)}$, assuming a singularity of the form given in (1.6).

We have seen in (1.7) that according to RG theory $\chi_0^{(2)}/\chi_0$ should be free of logarithmic factors and diverge at the critical point like a pole of order three. We find that the Dlog–Padé approximants to the $\chi_0^{(2)}/\chi_0$ series do have an isolated pole on the real positive v axis, characteristic of a simple algebraic singularity not complicated by logarithmic factors. The location of this pole and its corresponding residue as obtained from the diagonal and main off-diagonal approximants are given in table 2. In contrast to Baker (1977), who found that the series up to v^9 gave rise to an erratic Padé table, we find that with eight more series coefficients the last few table entries are very close indeed to the value of $1/v_c$ given in (2.5) with a residue around 2·98. This value for the exponent differs by only $\frac{2}{3}$% from the RG prediction.

Table 2. Dlog–Padé analysis of $\chi_0^{(2)}/\chi_0$ series for the $d=4$ Ising model.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	6·7561 (−2·9188)	6·7771 (−2·8930)	6·7884 (−2·8743)
3	6·8017 (−2·8407)	6·7781 (−2·8917)‡	6·7281 (−2·9895)
4	6·7647 (−2·9114)§	6·7301 (−2·9843)	6·7293 (−2·9867)
5	6·7286 (−2·9889)	6·7294 (−2·9862)	6·7293 (−2·9867)†
6	6·7241 (−2·9983)†	6·7307 (−2·9822)	6·7333 (−2·9695)
7	6·7318 (−2·9779)	6·7315 (−2·9790)	6·7314 (−2·9795)
8	6·7313 (−2·9799)	6·7316 (−2·9785)†	

† Defect on positive axis.
‡ Defect on negative axis.
§ Defect in complex plane.

We have also studied $\chi_0^{(2)}$ using Guttmann's method of analysis. We assume

$$\chi_0^{(2)} \sim t^{-4}|\ln t|^p \tag{3.1}$$

and try to determine the correction exponent p. We now take $q^*=4$ in (2.3) and analyse for a range of values of p^* for fixed $1/v_c^*$ equal to the central value in (2.5). (The uncertainties quoted in (2.5) do not affect our conclusions.) In contrast to the case of χ_0, the exponent estimates $n(R_n v_c^* - 1)$ possess considerable curvature when plotted against $1/n$, making it more difficult to estimate their limit. However, a small positive value of p^* is definitely preferred. Assuming $p^*=\frac{1}{3}$, as predicted by RG theory, gives the sequence

$$\begin{aligned} &-0{\cdot}531713(n=10), && -0{\cdot}513470(n=11), && -0{\cdot}495964(n=12),\\ &-0{\cdot}479284(n=13), && -0{\cdot}463460(n=14), && -0{\cdot}448484(n=15),\\ &-0{\cdot}434330(n=16), && -0{\cdot}420959(n=17). \end{aligned} \tag{3.2}$$

Analysis of this sequence using Neville tables (Gaunt and Guttmann 1974) indicates a limit close to zero. Also, the sequence R_n is found to be consistent with a horizontal approach to $1/v_c^*$, though rather slowly. We conclude, therefore, that the coefficients of $\chi_0^{(2)}$ can be fitted to a singularity of the form predicted by RG theory.

4. Conclusions

We have investigated high-temperature series expansions up to v^{17} for the zero-field susceptibility χ_0 and the fourth-field derivative of the free energy $\chi_0^{(2)}$ for the $d=4$ Ising model. The series have been analysed using a recent method due to Guttmann (1978) on the assumption that the physical singularity is of the form $t^{-q}|\ln t|^p$. For χ_0, we fixed q at its mean-field value of $q=1$ and then estimated $p=0{\cdot}33\pm0{\cdot}07$, in good agreement with the prediction $q=1, p=\frac{1}{3}$ of RG theory. For $\chi_0^{(2)}$, convergence is rather slower and we were unable to make a definite estimate of p having fixed q at its mean-field value, $q=4$. Instead we found that the series could be fitted quite well with a range of small positive values of p, including the RG value of $p=\frac{1}{3}$. Using Padé approximant techniques we have also found evidence that $\chi_0^{(2)}/\chi_0$ is logarithm-free as predicted by RG theory, and made the estimate $2\Delta\simeq2{\cdot}98$ in close agreement with the RG value of $2\Delta=3$.

In summary, we have not found any conflict between high-temperature series results and the predictions of RG theory for the $d=4$ Ising model. In our opinion, any small discrepancies which remain could be accounted for in terms of the finite number of coefficients available, slow convergence of successive approximation schemes, additive corrections to the dominant singular form (Baker and Golner 1977), and so on. This conclusion is contrary to that drawn by Baker (1977), although it should be added that his work was done with much shorter series.

In subsequent work we will examine the analogous situation below and at the critical temperature.

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