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COMMENT

The adiabatic susceptibility and specific heat at constant magnetisation of the Ising model

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Abstract. Low-temperature series expansions for the adiabatic susceptibility of the spin-$\frac{1}{2}$ Ising model in three dimensions are generated. A simple ratio analysis of the susceptibility coefficients on low-coordination lattices leads to the hypothesis that in the critical region $C_H/C_M = \chi_T/\chi_S \approx 4$.

The nature of the critical behaviour of the specific heat at constant magnetisation in zero field has received little attention. As pointed out in an earlier study by Baker and Gaunt (1967), the well-known thermodynamic relation in standard notation

$$C_H - C_M = T(\partial M/\partial T)_H^2(\partial H/\partial M)_T \tag{1}$$

implies that $C_M \leqslant C_H$. For $T > T_C$ and $H = 0$ equation (1) implies that $C_M = C_H$ for all models. In mean field theory $C_M/C_H = 0$ for $T < T_C$. In the two-dimensional spin-$\frac{1}{2}$ Ising model (Baker and Gaunt 1967)

$$C_M/C_H \approx 1 + E/\ln(1 - T/T_C), \qquad T \to T_C^-, \tag{2}$$

where the slightly lattice-dependent amplitude $E \approx 1{\cdot}8$.

For the three-dimensional Ising model one might expect the asymptotic ratio of C_M/C_H to lie somewhere between the mean field and two-dimensional results. From the then available low-temperature series expansions Baker and Gaunt derived series for C_M/C_H and concluded that $C_M/C_H \approx 1$ also for the three-dimensional Ising model.

Because of the well-known thermodynamic relation

$$C_M/C_H = \chi_S/\chi_T, \tag{3}$$

where χ_S and χ_T are the adiabatic and isothermal susceptibilities, one may equally well study susceptibility series. For the specific heat at constant field, the spontaneous magnetisation and the initial isothermal susceptibility of the spin-$\frac{1}{2}$ Ising model low-temperature expansions in u of very considerable length are now available on five regular cubic lattices. The lengths of the series are listed in table 1. For the first four lattices the data were derived by Sykes *et al* (1965, 1973a) and for the hydrogen peroxide lattice by Betts *et al* (1974).

Analysis of the spontaneous magnetisation series was quite successful; the initial isothermal susceptibility series proved difficult to analyse, and the analysis of the constant field specific heat series was almost completely unsuccessful (Gaunt and Sykes 1973, Betts and Chan 1974).

Table 1. Maximum degree of published low-temperature series for the Ising model.

Lattice	FCC	BCC	SC	Diamond	Hydrogen peroxide
Coordination number	12	8	6	4	3
Maximum degree	40	28	20	15	17

We have derived series for $\chi_S = \Sigma_n c_n^S u^n$ and $C_M/Nk_B (\log u)^2 = \Sigma_n a_n^S u^n$ on all five three-dimensional lattices. We have assumed power-law singularities of the standard form

$$\chi_S \approx C'_S(1 - T/T_C)^{-\gamma'_S}, \qquad H = 0, \quad T < T_C \tag{4}$$

and

$$C_M \approx A'_M(1 - T/T_C)^{-\alpha_M}. \tag{5}$$

From (1) and (3) $\gamma'_S \leqslant \gamma'$ and $\alpha'_M \leqslant \alpha'$. The series for C_M, like those for C_H, are completely intractable to standard ratio and Padé approximant methods of analysis. We have analysed the series for χ_S by the standard ratio and Padé approximant methods. They are better behaved than the specific heat series, but somewhat worse behaved than the corresponding series for χ_T. In summary we have not learned much from direct analysis of the series and thus we omit any details for C_M and χ_S.

For the SC, BCC and FCC lattices the coefficients in the low-temperature series for all thermodynamic properties of the Ising model are irregular in sign; for the diamond and hydrogen peroxide lattices, however, all coefficients are of the same sign. The coefficients c_n^S for the latter two lattices are listed in table 2. In figure 1 we have plotted

Table 2. Coefficients of the low-temperature expansion of the reduced adiabatic susceptibility, $\chi_S = k_B T(\partial^2 M/\partial H^2)_S/(g\mu_B)^2 N$, for the spin-$\frac{1}{2}$ Ising model.

Degree	Lattice	
n	Diamond	Hydrogen peroxide
0	0	0
1	0	0
2	0	0
3	2	0
4	15	2·666666667 . . .
5	78·5	14·22222222 . . .
6	429·75	58·9629629 . . .
7	2188·625	215·5061728 . . .
8	11022·9375	732·6748971 . . .
9	54058·40625	2380·159122 . . .
10	258711·6094 . . .	7794·977595 . . .
11	1224155·414 . . .	26259·50922 . . .
12	5726839·121 . . .	90006·40187 . . .
13	26559135·68 . . .	307104·4959 . . .
14	122583321·0 . . .	1029648·168 . . .
15	563722867·8 . . .	3390131·321 . . .
16		11041033·85 . . .
17		35870974·20 . . .

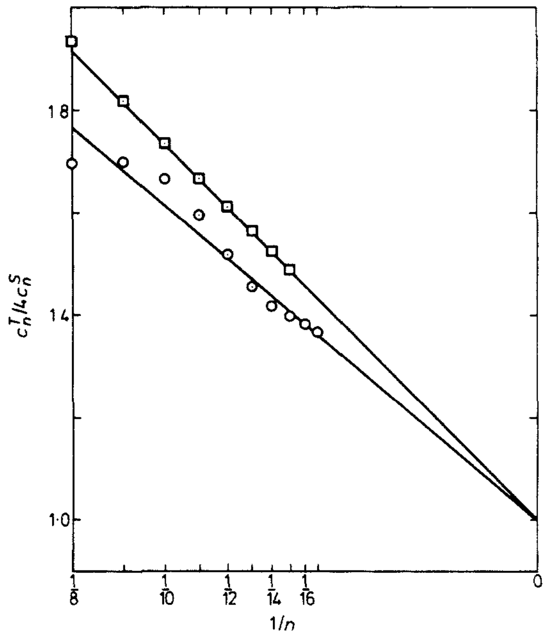

Figure 1. Ratios of coefficients $c_n^T/4c_n^S$ of corresponding powers in the low-temperature expansions of the isothermal susceptibility χ_T and adiabatic susceptibility χ_S of the Ising model on the diamond lattice (squares) and hydrogen peroxide lattice (circles) against $1/n$.

for the latter two lattices the ratio of coefficients $c_n^T/4c_n^S$ for corresponding powers of the independent variable in the series for χ_T and χ_S. (For the hydrogen peroxide lattice the independent variable is $z = \exp(-2J/kT)$ and for the diamond lattice is $u = z^2$.)

The diamond lattice ratios are very linear in $1/n$. By extrapolation we estimate $c_n^T/c_n^S \approx 4{\cdot}00 \pm 0{\cdot}05$ as $n \to \infty$. The ratios for the hydrogen peroxide lattice have a pronounced oscillation which seems to be damping out for higher n. For the hydrogen peroxide lattice we estimate that $c_n^T/c_n^S \approx 4{\cdot}0 \pm 0{\cdot}5$. There is no clear evidence for q dependence of c_n^T/c_n^S.

To test the above method we have also computed the adiabatic susceptibility of the Ising model on the honeycomb lattice using the basic data of Sykes *et al* (1973*b*). For this two-dimensional lattice we expect from (2) and (3) that $c_n^T/c_n^S \approx 1$ as $n \to \infty$. However, because of expected logarithmic corrections this limit may be indicated numerically only by rather long series. Like the ratios for the hydrogen peroxide lattice, c_n^T/c_n^S for the honeycomb lattice show oscillations. On the basis of the available data we estimate that $c_n^T/c_n^S \approx 1{\cdot}4 \pm 0{\cdot}4$, which is not inconsistent with the exact asymptotic limit of unity.

The thermodynamic relation (1) admits of three separate cases of critical behaviour. (*a*) The first and third terms diverge more strongly than the second. The Rushbrooke (1963) inequality becomes the scaling equality

$$\alpha' + 2\beta + \gamma' = 2, \tag{6a}$$

and the inequality

$$\gamma' > \gamma \tag{6b}$$

holds. (*b*) The first and second terms diverge more strongly than the third, so that the Rushbrooke inequality becomes

$$\alpha' + 2\beta + \gamma' > 2, \tag{7a}$$

and the equality

$$\gamma' = \gamma'_S \tag{7b}$$

is valid. (*c*) All three terms diverge equally strongly. Then both equalities (6*a*) and (7*b*) hold. Case (*c*) holds for the two-dimensional Ising model and, it now seems, also for the three-dimensional Ising model.

On the basis of the above evidence we conjecture further that for the three-dimensional $S = \frac{1}{2}$ Ising model

$$\chi_S/\chi = C_M/C_H \approx \tfrac{1}{4}. \tag{8}$$

More sophisticated analysis of the series, particularly for the higher-q lattices, could either strengthen or disprove this conjecture.

I would like to thank Professor John Stephenson for a helpful discussion. Dr R Gourishankar provided assistance with the numerical calculations.

Note added in proof. A D Bruce (1979, private communication) has just shown, on the basis of earlier renormalisation group investigations by Aharony and Hohenberg (1976), that χ_S/χ_T approaches a constant in the critical region within each universality class. Bruce has further shown that this result is particularly significant for the interpretation of experiments on ferroelectrics. I am grateful to Dr Bruce for informing me of these results prior to their publication.

References

Aharony A and Hohenberg P C 1976 *Phys. Rev.* B **13** 3081–90
Baker G A Jr and Gaunt D S 1967 *Phys. Rev.* **155** 545–52
Betts D D and Chan C F S 1974 *J. Phys. A: Math., Nucl. Gen.* **7** 650–64
Betts D D, Elliott C J and Sykes M F 1974 *J. Phys. A: Math., Nucl. Gen.* **7** 1323–34
Gaunt D S and Sykes M F 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1517–26
Rushbrooke G S 1963 *J. Chem. Phys.* **39** 842
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283–98
Sykes M F, Gaunt D S, Essam J W and Elliott C J 1973a *J. Phys. A: Math., Nucl. Gen.* **6** 1507–16
Sykes M F, Gaunt D S, Martin J L, Mattingly S R and Essam J W 1973b *J. Math. Phys.* **14** 1071–4