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Critical parameters for the heat capacity of three-dimensional Ising ferromagnets

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Abstract. The singularity of the heat capacity for the spin-$\frac{1}{2}$ Ising ferromagnet arrayed on simple cubic and diamond lattices is investigated through the analysis of high-precision Monte Carló data for the internal energy. The analysis incorporates confluent singularities. Two least-squares fitting procedures are considered. In the first one, the leading confluent singularity amplitude is zero and the next confluent singularity is included. For both lattices this procedure gives accordance with: (i) the universal value for the ratio of the leading singularity amplitudes predicted from the ε expansion and (ii) the theoretical expectation of equality between the non-singular parts of the heat capacity above and below the critical temperature. In the second least-squares fitting procedure, the leading confluent singularity is finite. This leads to a fit which disagrees with both (i) and (ii). The Monte Carlo results suggest that the failure of the series analysis to accord with (i) and (ii) may be due to neglect of a rather large confluent singularity in the ferromagnetic phase.

1. Introduction

The critical properties of the three-dimensional Ising ferromagnet have been studied in great detail by analysis of series expansions (see e.g. Domb 1974). By and large the results are consistent with the universal properties predicted from other theoretical approaches such as the ε expansion (Brézin *et al* 1976). However, there seems to be one case where a rather substantial disagreement exists, namely the case of the heat capacity.

Close to the critical temperature T_c it is expected that the heat capacity has the form (Barmatz *et al* 1975)

$$C(t)=\begin{cases}A^+t^{-\alpha}(1+D^+t^{\Delta}+F^+t^{2\Delta})+B^+ & T>T_c\\ A^-(-t)^{-\alpha}(1+D^-(-t)^{\Delta}+F^-(-t)^{2\Delta})+B^- & T<T_c\end{cases}\tag{1}$$

where $t=(T-T_c)/T_c$. $\alpha=0.125$ and $\Delta=0.493$ (le Guillou and Zinn-Justin 1977) for a three-dimensional system with Ising symmetry.

It is expected theoretically (Wegner 1976) that the non-singular part of C is symmetric, i.e.

$$B^+=B^-.\tag{2}$$

So far, the diamond lattice is the only three-dimensional lattice where series analysis has given estimates for both B^+ and B^-. High-temperature series leads to $B^+=-1.23$

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(Hunter 1967, Domb 1974) and low-temperature series gives $B^- = -0.13$ (Gaunt and Domb 1968). Obviously, these numbers are not in accordance with (2). Furthermore, the ratio of the leading singularity amplitudes, A^+/A^-, is universal and has been calculated by the ε-expansion technique. The result for a system with Ising symmetry is 0.55 to first order in ε (Brézin *et al* 1974) and 0.48 to second order (Bervillier 1976). The series analysis leads to a somewhat larger value of 0.63 for the simple cubic lattice (Fisher and Tarko 1975) and 0.75 for the diamond lattice (Gaunt and Domb 1968). Consequently, it seems desirable to investigate the critical behaviour of the heat capacity by an alternative approach.

In this paper we report a study of the Ising ferromagnet, where the Monte Carlo method is used to obtain 'experimental' data which are analysed to give the parameters in (1). Actually, it is advantageous to study the energy rather than the heat capacity because the statistical error on the energy is roughly an order of magnitude smaller than the error on the heat capacity. Close to T_c the energy varies as

$$E(t) = \begin{cases} E_c + E_1^+ t^{1-\alpha} + E_2^+ t + E_3^+ t^{1-\alpha+\Delta} + E_4^+ t^{1-\alpha+2\Delta} & T > T_c \\ E_c + E_1^- (-t)^{1-\alpha} + E_2^- (-t) + E_3^- (-t)^{1-\alpha+\Delta} + E_4^- (-t)^{1-\alpha+2\Delta} & T < T_c \end{cases} \qquad (3)$$

where the parameters $E_i^\pm$, $i = 1, \ldots, 4$, are simply related to the parameters in (1), and E_c denotes the energy at T_c. It might be expected that the advantage of working with the more accurate energy data rather than the heat capacity may be offset by increased difficulties in the data analysis due to the additional parameter E_c in (3) relative to (1). This is not the case, however, as E_c may be determined independently from finite size considerations as described in § 2.

A less extensive Monte Carlo investigation of the heat capacity for a spin-$\frac{1}{2}$ Ising ferromagnet on a simple cubic lattice has already been reported (Landau 1976). Various fitting procedures of $C(t)$ were considered. However, accordance of A^+/A^- with the ε-expansion result was obtained only by a constrained fitting procedure, where both B^+ and B^- were set equal to the value derived from high-temperature series analysis. This constraint is not imposed in our study.

Our calculations are performed for the Ising ferromagnet arrayed on a diamond lattice and on a simple cubic lattice. For both lattices the results are consistent with (2) and with the value for A^+/A^- predicted by the ε expansion, provided the leading confluent singularity is absent, i.e. $D^+ = D^- = 0$. The paper is organised as follows. In § 2 we describe the Monte Carlo calculations and in § 3 we present the results of the analysis of the Monte Carlo data. Finally, in § 4 we discuss our results.

2. Monte Carlo calculations

We consider a simple cubic lattice and a diamond lattice with N^3 and $4 \times N^3$ lattice points, respectively. Both lattices are of cubical form with toroidal periodic boundary conditions. A spin $\sigma_j = \pm 1$ is placed at each lattice point and the interaction between the spins is given by

$$H = -J \sum_{\langle j,k \rangle} \sigma_j \sigma_k \qquad J > 0$$

where the summation extends over all nearest neighbours of spins.

The energy is calculated for a number of temperatures by a conventional Monte Carlo importance sampling method. To improve the statistics we have, for each temperature, performed the Monte Carlo calculations at least three times starting from different equilibrium configurations of the spins. The energy is obtained as the average of the energy estimate from the different calculations and the error ΔE is determined as the root-mean square deviation. Typically, $\Delta E/E$ is below 2×10^{-3}.

It is well known that finite size effects are important close to T_c, when the correlation length $\xi(t)$ becomes comparable to the lattice length, N. For periodic boundary conditions the finite-size effects on the energy are given by (see e.g. Binder 1979)

$$E(t, N)-E(t, N=\infty) \propto \exp(-N/\lambda(t)) \qquad t\neq 0 \tag{4}$$

$$E(t=0, N)-E(t=0, N=\infty) \propto N^{-(1-\alpha)/\nu} \qquad t=0 \tag{5}$$

where $\lambda(t)$ is proportional to $\xi(t)=\xi_0 t^{-\nu}$. We have ensured that finite-size effects are unimportant for $t\neq 0$ by performing additional calculations on a larger lattice. The data are only accepted if the two calculations give the same value for the energy within the estimated error. The number of spins varies from 8000 to 108 000. The data are obtained with a uniform density in the interval $6\times10^{-3}\leqslant|t|\leqslant3\times10^{-1}$. The consistency of the data is checked by observing accordance with the known high-temperature series for $t\geqslant0.25$ (Domb 1974).

To reduce the number of unknown parameters in (3), we have performed Monte Carlo calculations at T_c for a number of different lattice sizes. The value of T_c is taken from the series analysis†. The data obtained, $E(t=0, N)$, fit (5) for $N\geqslant16$, and the extrapolated values of $E_c=E(t=0, N=\infty)$ are given in table 1 together with the values derived from series analysis. It appears from table 1 that the Monte Carlo estimate for E_c is consistent with the series analysis estimate in the case of the simple cubic lattice, whereas the two estimates differ by approximately 1% for the diamond lattice.

Table 1. Critical energies E_c in units of J.

	Diamond	Simple cubic
Monte Carlo calculations	-0.865 ± 0.002[a]	-0.990 ± 0.004[a]
Series analysis	-0.874 ± 0.005[b]	-0.99218 ± 0.00015[c]

[a] This work.
[b] Hunter (1967).
[c] Sykes *et al* (1972).

3. Data analysis

The parameters in (3) are derived by least-squares fitting of (3) to the energy data. This turns out not to be a simple task as the smallness of α makes the simultaneous determination of $E_1^{\pm}$ and $E_2^{\pm}$ an almost degenerate problem. As already mentioned, E_c has been determined independently and is thus a constant in the least-squares fitting. T_c is $(4.5108\pm0.0002)J/k_B$ for the simple cubic lattice (Sykes *et al* 1972) and $(2.7042\pm0.0002)J/k_B$ for the diamond lattice (Gaunt and Sykes 1973). The uncertainty of T_c is of no importance in the t interval covered by our data.

† We have refrained from estimating T_c from Monte Carlo calculations since it is known with greater accuracy from series analysis than may conceivably be obtained from Monte Carlo calculations.

Table 2. Parameters $E_i^{\pm}$, $i = 1, \ldots, 4$, in (3). I, Parameters estimated from a least-squares fit of (3) with $E_4^+ = E_4^- = 0$; II, parameters estimated from a least-squares fit of (3) with $E_3^+ = E_3^- = 0$; SA, parameters estimated from series analysis.

		E_1^+	E_2^+	E_3^+	E_4^+	E_1^-	E_2^-	E_3^-	E_4^-
I	Diamond	3.91 ± 0.16	-3.94 ± 0.26	0.54 ± 0.11		-5.01 ± 0.60	-0.6 ± 1.1	5.17 ± 0.75	
	Simple cubic	6.32 ± 0.13	-6.59 ± 0.18	0.90 ± 0.06		-9.6 ± 2.2	1.7 ± 4.2	6.4 ± 3.0	
II	Diamond	3.61 ± 0.27	-3.36 ± 0.38		0.40 ± 0.26	-6.55 ± 0.67	2.9 ± 1.1		5.4 ± 1.6
	Simple cubic	5.61 ± 0.33	-5.33 ± 0.44		0.48 ± 0.25	-11.91 ± 0.90	6.7 ± 1.5		5.8 ± 2.5
SA	Diamond	3.62[a]	−3.33[a]			−4.94[b]	0.352[b]		
	Simple cubic	5.856[c]	−5.602[c]			−9.48 ± 0.54[d]			

[a] Hunter (1967).
[b] Gaunt and Domb (1968).
[c] Sykes *et al* (1972).
[d] Fisher and Tarko (1975).

We have performed two three-parameter fits, one with $E_4^+ = E_4^- = 0$ and one with $E_3^+ = E_3^- = 0$. The motivation for the latter fit stems from the fact that series studies of the Ising ferromagnet on a face centred cubic lattice indicate that the leading singularity amplitude vanishes for spin-$\frac{1}{2}$ systems (Camp *et al* 1976).

The analysis is performed for a number of E_c values within the estimated error interval. Only fits for which the parameters stay stable over a temperature interval are accepted. In table 2 we give the values of the resulting parameters. The errors are estimated from the variation of the parameters with E_c. It should be noted that the quality of the two sets of fits is equally good.

Table 2 shows that the relation $E_2^+ = -E_2^-$, which is equivalent to (2), is supported by the results only when E_3^+ and E_3^- have been set to zero. The ratio, $-E_1^+/E_1^-$, which is identical to A^+/A^-, is given in table 3. It appears that accordance with the ratio predicted by the ε expansion is obtained only for the case with $E_3^+ = E_3^- = 0$. Consequently, the analysis of the Monte Carlo data supports the relation given in (2) and the value for A^+/A^- predicted from the ε expansion, provided the leading confluent singularity is absent and that the next confluent singularity is considered. It might be expected that a four-parameter fit containing the first as well as the second confluent singularity would be useful in showing whether $E_3^\pm$ were in fact zero. It turns out however, that such a fit has too many degrees of freedom to lead to a stable fit.

Table 3. Estimates of the ratio of the leading singularity amplitudes for the heat capacity, $-E_1^+/E_1^-(=A^+/A^-)$ in (3). I and II refer to the ratio obtained from the two fits in table 2.

	I	II	Series analysis	ε expansion
Diamond	0.79 ± 0.13	0.56 ± 0.10	0.75[a]	0.55[c], 0.48[d]
Simple cubic	0.70 ± 0.17	0.48 ± 0.06	0.63[b]	

[a] Gaunt and Domb (1968).
[b] Fisher and Tarko (1975).
[c] First order in ε (Brézin *et al* 1976).
[d] Second order in ε (Bervillier 1976).

4. Discussion

Our analysis attempts to determine the linear parameters in the expression for the heat capacity close to T_c. The functional forms of the heat capacity and the energy are too smooth in the $|t|$ interval (down to $|t| = 6\times10^{-3}$) covered in our study to make any attempt at determining also the exponents α and Δ nothing but an exercise in futility. Therefore we fix the exponents at the literature values. T_c is also taken from the literature. Since T_c may be obtained with great accuracy in series analysis, the small error quoted is of no importance in our study. The smoothness of the energy curve makes it impossible with our data to prefer least-squares fits involving a leading confluent singularity to fits where the leading confluent singularity is replaced by the next confluent singularity. Only in the latter case is agreement obtained with the relation in (2) and with the ε-expansion prediction of A^+/A^-. This observation applies for both the simple cubic lattice and for the diamond lattice.

Table 2 allows a comparison of our estimate for $E_1^\pm$ and $E_2^\pm$ with the corresponding series analysis estimates. The agreement between the two sets is quite good for $T > T_c$ in the case where the leading confluent singularity is absent. For $T < T_c$ the agreement is less good. This suggests that the failure of the series analysis to agree with the ε expansion upon the value of A^+/A^- may be due to shortcomings of the low-temperature expansion. It appears that the values of E_4^- (and E_3^-) are comparable to E_1^- but of opposite sign. The series analysis did not take confluent singularities into account and the relatively large value for E_4^- (and E_3^-) may lead to misleading estimates for E_1^- unless the series is very long.

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