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Heat capacity of the $S = \infty$ Ising ferromagnet studied by Monte Carlo simulation

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Abstract. The heat capacity of the $S = \infty$ Ising ferromagnet arrayed on a simple cubic lattice is investigated by analysis of Monte Carlo data for the internal energy. A function is least-squares fitted to the energy data close to the critical temperature T_c. The function is consistent with the expected singularity of the heat capacity $C(t) = A^{\pm}|t|^{-\alpha}[1 + D^{\pm}|t|^{\Delta_1}] + B^{\pm}$, where $t = (T - T_c)/T_c$ and the $\pm$ superscripts refer to $t > 0$ and $t < 0$, respectively. The results of the data analysis show that the relation $B^+ = B^-$ is supported and that A^+/A^- accords with the expected universal value for a system with Ising symmetry. The ratio of the confluent singularity amplitudes D^+/D^- is somewhat lower than the expected universal value. The amplitudes of the leading and confluent singularities of the order parameter are reported also.

1. Introduction

Close to the critical temperature T_c the heat capacity of the Ising ferromagnet is expected to vary with temperature as

$$C(t) = \begin{cases} A^+t^{-\alpha}[1 + D^+t^{\Delta_1} + F^+t^{\Delta_2}] + B^+ & T > T_c \\ A^-(-t)^{-\alpha}[1 + D^-(-t)^{\Delta_1} + F^-(-t)^{\Delta_2}] + B^- & T < T_c \end{cases} \tag{1}$$

where $t = (T - T_c)/T_c$. Usually, $A^{\pm}|t|^{-\alpha}$ is referred to as the leading singularity and $D^{\pm}|t|^{\Delta_1}$ as the leading confluent singularity. Recently, $C(t)$ has been studied in the $S = \frac{1}{2}$ case by analysis of energy data derived from Monte Carlo (MC) simulations (Knak Jensen and Mouritsen 1982). This analysis indicates that accordance of A^+/A^- with the expected universal value is obtained only provided the leading confluent singularity vanishes. Some high-temperature series analyses (Camp *et al* 1976) suggest that D^+ is zero for $S = \frac{1}{2}$, whereas analysis of longer series indicates that D^+ is finite for $S = \frac{1}{2}$ (Nickel 1981). Series analysis for general S gives evidence that the amplitude vanishes for S between 1 and 2 (Zinn–Justin 1981).

Since the analysis of MC data fails to accord with the universal value for A^+/A^- in the presence of a confluent singularity for $S = \frac{1}{2}$ it is useful to investigate whether this is the case in general or whether it is restricted to $S = \frac{1}{2}$. This paper reports an investigation of the $S = \infty$ Ising ferromagnet arrayed on a simple cubic lattice by the same method as used for the $S = \frac{1}{2}$ case. The method utilises the energy rather than $C(t)$ since the former has a much smaller statistical error than the latter (a fluctuation

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quantity). Close to T_c the energy varies as

$$E(t)=\begin{cases} E_c+E_1^+t^{1-\alpha}+E_2^+t+E_3^+t^{1-\alpha+\Delta_1}+E_4^+t^{1-\alpha+\Delta_2}+\ldots & T>T_c \\ E_c+E_1^-(-t)^{1-\alpha}+E_2^-(-t)+E_3^-(-t)^{1-\alpha+\Delta_1}+E_4^-(-t)^{1-\alpha+\Delta_2}+\ldots & T<T_c. \end{cases} \tag{2}$$

The parameters $E_i^\pm$, $i=1,\ldots 4$, are simply related to the parameters in (1). The additional parameter E_c—the critical energy—in (2) relative to (1) may be estimated from finite-size analysis (see e.g. Binder 1979) using

$$E(t=0,N)-E_c \propto N^{-(1-\alpha)/\nu}, \tag{3}$$

where $E(t=0,N)$ denotes the energy for a system with N^3 spins at $T=T_c$.

It turns out that a data analysis incorporating a confluent singularity leads to accordance of A^+/A^- with the universal value in the $S=\infty$ case. This agreement makes it meaningful to investigate if the analysis leads to accordance also with the universal value for D^+/D^-. The analysis shows that the derived value for D^+/D^- is lower than the value expected theoretically. An analysis performed on constructed 'data' suggests that the disagreement is related to higher-order correction terms, which cannot easily be handled in the analysis, due to insufficient accuracy of the MC data.

The paper is organised as follows. In § 2 the model and some of the computational details are presented. Section 3 describes the analysis of the MC data for the energy, both for $t=0$ and $t\neq 0$. This section also contains an analysis of the order parameter, which is obtained as a by-product of the MC calculations. Finally, the results are discussed in § 4.

2. Model and computational details

The $S=\infty$ Ising ferromagnet is defined by the Hamiltonian

$$\mathscr{H}=-J\sum_{\langle j,k\rangle} S_{jz}S_{kz} \qquad J>0 \tag{4}$$

where $\langle j,k\rangle$ indicates a nearest-neighbour pair and S_{jz} is the z-component of a classical vector $\boldsymbol{S}_j=(S_{jx},S_{jy},S_{jz})$ of unit length. The x and y components do not interact but merely act as a reservoir for fluctuations. The model (4) is arrayed on a simple cubic lattice of cubical form of size $L=N^3$ with periodic boundary conditions.

A conventional Monte Carlo importance sampling simulation is used to derive the internal energy $E=\langle\mathscr{H}\rangle$ and the order parameter $M=L^{-1}\langle|\sum_{j=1}S_{jz}|\rangle$. The simulations are performed for a number of temperatures selected to resemble a uniform distribution in $\ln(|t|)$ and to be symmetric around $t=0$. In all, 46 temperatures are considered. The smallest value of $|t|$ is 6×10^{-3}. Finite-size effects are important when the correlation length of the system becomes comparable to the linear dimension N of the lattice. These effects are avoided by checking that the data are insensitive to an increase in lattice size. The largest lattice considered has a linear dimension of $N=40$. All data are obtained as an average of at least three simulations starting from different initial configurations of the spins. The error of the data ΔE is estimated as the root-mean square deviation. The relative errors $\Delta E/E$ are typically 2×10^{-3} and 10^{-2} for $t\neq0$ and $t=0$, respectively. Similarly, the magnetisation data has typically a relative error of 2×10^{-3}.

3. Results

3.1. Data analysis for $t = 0$

The energy is calculated for a number of different lattice sizes at $T = T_c = 1.6639\ J/k_B$, which is the estimate for the critical temperature derived from analysis of high-temperature series (Camp and Van Dyke 1975). The data $E(t=0, N)$ are used to determine E_c using (3). In this analysis the exponent $(1-\alpha)/\nu$ is set to 1.413 ± 0.004 based on $\nu = 0.6300 \pm 0.0015$ (Le Guillou and Zinn–Justin 1980) and $2 - \alpha = d\nu$, where d is the spatial dimension. It is found that the data may be represented by

$$E(t=0, N) = E_c + pN^{-(1-\alpha)/\nu} \tag{5}$$

for N ranging from 40 to 10 with

$$E_c = -0.385 \pm 0.03 \qquad \text{and} \qquad p = -1.08 \pm 0.09. \tag{6}$$

Figure 1 shows the data and the line given by (5) and (6). The limits of error on E_c and p are calculated from the statistical error on the data and the limit of error of ν. An error ΔT_c in the estimate of T_c has not been included. ΔT_c is not reported in the literature. If ΔT_c is set to 2×10^{-4} the contribution to the limit of error on E_c is approximately 2×10^{-3}.

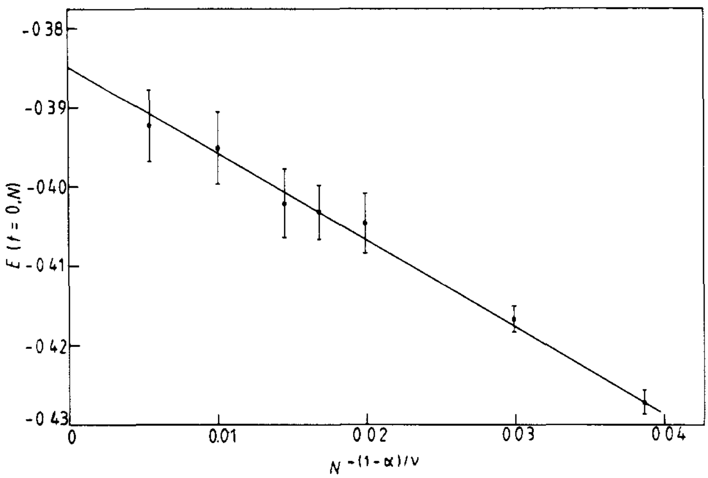

Figure 1. Energy for the $S = \infty$ Ising ferromagnet arrayed on a simple cubic lattice with N^3 spins calculated at $T_c = 1.6639\ J/k_B$ ($t = 0$). The line is obtained from a least-squares fit and is represented by $E(t=0, N) = -0.385 - 1.09\ N^{-1\ 413}$.

3.2. Data analysis for $t \neq 0$

The least-squares fitting of (2) to the data involves in principle a large number of parameters to be determined, $E_i^{\pm}$, the critical exponents and T_c. Moreover, there may be additional confluent singularities (Rehr 1979). All these parameters cannot be extracted from the data. Instead the strategy is adopted to fix the exponents and T_c at the literature values and determine the unknown linear parameters, $E_i^{\pm}$. Specifically, the exponents are set to $\alpha = 0.11$ and $\Delta_1 = 0.498$ (Le Guillou and Zinn–Justin 1980).

Least-squares fits are only accepted if the parameters stay reasonably constant over an interval.

The simplest analysis considered is to fit (2) with $E_4^+ = E_4^- = 0$ for $T > T_c$ and $T < T_c$, separately, to the data for a number of different E_c values within the interval in (6). Stable fits are obtained only for $-0.388 \leqslant E_c \leqslant -0.385$. The derived values for $E_i^\pm$ are given in table 1. It appears from this table that $-E_1^+/E_1^- = A^+/A^- = 0.55 \pm 0.21$ accords with the theoretical estimates of 0.55 (Brézin *et al* 1976) and 0.48 (Bervillier 1976) obtained to first and second order in $\varepsilon(=4=d)$, respectively. Furthermore, the relation $B^+ = B^-(E_2^+ = -E_2^-)$ is supported by the data in table 1.

Table 1. Parameters $E_i^\pm$, $i = 1, 2$, and 3 in (2) estimated from a least-squares fit with $E_4^+ = E_4^- = 0$, $\alpha = 0.11$ and $\Delta_1 = 0.498$. A plus (minus) superscript indicates $T > T_c(T < T_c)$.

	$E_1^\pm$	$E_2^\pm$	$E_3^\pm$
$T < T_c$	-7.7 ± 0.7	3.9 ± 1.2	1.3 ± 0.7
$T > T_c$	4.1 ± 1.2	-4.2 ± 2.2	0.1 ± 1.5

A more comprehensive analysis including the $E_4^\pm$ terms (a four parameter fit) does not lead to stable fits. It is more useful to reduce the number of parameters to be determined. It is actually possible to make such a reduction and still retain a confluent singularity. This is achieved by fitting (2) simultaneously for $T > T_c$ and $T < T_c$ and imposing the constraint $-E_2^+ = E_2^- \equiv E_2$. This analysis contains five parameters $E_1^\pm$, $E_3^\pm$, and E_2. (E_1^+, E_3^+) and (E_1^-, E_3^-) are determined only from the data for $T > T_c$ and $T < T_c$, respectively, whereas E_2 is determined from all the data, so the analysis is in a way a two and a half parameter fit. The results are given in table 2. The data in tables 1 and 2 accord, but the estimated limits of error are much smaller in the latter table due to the imposed constraint.

Table 2. Parameters $E_i^\pm$, $i = 1, 2$, and 3 in (2) estimated from a least-squares fit with $E_4^+ = E_4^- = 0$, $\alpha = 0.11$ and $\Delta_1 = 0.498$. The least-squares fit is imposed the constraint $-E_2^+ = E_2^- = E_2$.

E_1^+	E_2	E_3^+	E_1^-	E_3^-
4.14 ± 0.16	4.30 ± 0.30	0.08 ± 0.43	-7.96 ± 0.21	1.15 ± 0.30

The ratio A^+/A^- may be estimated directly from the analysis by following its variation as the $|t|$-region is increased up to $|t_{max}| \sim 0.10$. It turns out that A^+/A^- fluctuates less than E_1^+ and E_1^-, individually, implying a correlation between E_1^+ and E_1^-. The ratio is estimated to

$$A^+/A^- = 0.521 \pm 0.014 \tag{7}$$

which agrees well with the theoretical estimate.

Least-squares fits have also been performed for α fixed at the extrema of its confidence interval, i.e. $\alpha = 0.1055$ and $\alpha = 0.1145$ (Le Guillou and Zinn-Justin 1980). The root-mean square derivation is as small as for $\alpha = 0.1100$. However, the parameters (except E_3^+) vary by 7–15%, whereas A^+/A^- varies 3–4%. Thus it appears that a slightly wrong value for α does not change the accordance of A^+/A^- with the universal value. This is in line with the idea that effective exponents obey scaling (Aharony and Ahlers 1980). Similarly, A^+/A^- is still in accordance with the universal value when T_c is varied within its assumed confidence interval of 2×10^{-4}. The accordance is preserved also if Δ_1 is shifted ±0.02 (Le Guillou and Zinn–Justin 1980).

3.3. *Confluent singularities*

It has been shown that the ratio of the confluent singularity amplitudes $D^+/D^-[=E_1^-E_3^+/(E_1^+E_3^-)]$ is universal (Aharony and Ahlers 1980, Chang and Houghton 1980). A series valid for a general symmetry n has been derived to second order in ε (Chang and Houghton 1980). For a system with Ising symmetry ($n=1$) the series is

$$D^+/D^-=1+1.15\varepsilon-4.56\varepsilon^2, \tag{8}$$

which obviously is unsuited to direct extrapolation to $\varepsilon=1$. However, a Padé approximant suggests $D^+/D^-\sim1.23$. Good agreement with the universal value has been found for CO_2 ($n=1$) (Greer and Moldover 1981) and for ^4He ($n=2$) (Mueller *et al* 1976). In other cases the sign of D^+/D^- is found to be negative (Bloemen *et al* 1980, Kallback *et al* 1981).

The data in table 1 lead to an estimate for $D^+/D^-\sim2.7\pm4.0$ which accords with the universal value, however, the limits of error are so large that the result deserves little merit. The constrained least squares fitting with $\alpha=0.1100$ and $\Delta_1=0.498$ leads to an estimate $D^+/D^-=-0.20\pm0.82$, which disagrees with the universal value. Variation of α and Δ_1 by the same amounts as described above does not lead to accordance either, although $\alpha=0.1145$ favours a larger value for D^+/D^-.

The origin of the lack of agreement is investigated by analysing a set of constructed 'data', derived from (2) with the following parameters; (i): $E_1^\pm$, E_2, and E_3^- are close to the values in table 2, (ii): E_3^+ is given a value consistent with the universal value D^+/D^-, (iii): $E_4^+=-E_3^+$, (iv): $E_4^-=\frac{1}{2}$, and (v): $\Delta_2=2\Delta_1$. The constructed 'data' are calculated at the same t-values as used in the MC simulations, and they are given a random error of the same magnitude as pertains to the MC data. The 'data' are analysed with the constrained fitting procedure, which neglects the E_4-terms. The analysis uses the same values for T_c, α and Δ_1 as employed in constructing the 'data'. The results show that the derived values of $E_1^\pm$ and E_2 agree well with the input values, whereas $E_3^\pm$ becomes some sort of average of the input values of $E_3^\pm$ and $E_4^\pm$. The estimate for D^+/D^- is lower than the universal value by 63%. This suggests that the neglect of higher-order corrections in the analysis of the MC data may be a major cause for the low value obtained for D^+/D^-. Obviously, it is desirable to include the E_4-terms in the constrained least-squares analysis. However, the smoothness of $E(t)$ combined with the insufficient accuracy of the data lead to an unstable fit.

3.4. *Analysis of order parameter data*

The expected functional form for the order parameter

$$m(|t|)=m_0(-t)^\beta[1+m_1(-t)^{\Delta_1}+m_2(-t)^{\Delta_2}] \qquad t<0 \tag{9}$$

is least-squares fitted to the data. The exponents are set to $\beta=0.3250\pm0.0015$ and $\Delta_1=0.498\pm0.020$ (Le Guillou and Zinn–Justin 1980). The analysis is performed first without the $m_2(-t)^{\Delta_2}$ term. It is found that (9) represents the data for $6\times10^{-3}\leqslant -t\leqslant 0.15$ with

$$m_0 = 1.164 \pm 0.010 \qquad \text{and} \qquad m_1 = -0.12 \pm 0.02. \tag{10}$$

The limits of error in (10) stem from the uncertainties in the exponents. The above analysis is performed for $T_c = 1.6639 J/k_B$. If T_c is shifted by $\pm 2\times10^{-4}$ the least-squares fits become poorer, suggesting that the reported value for T_c may be fairly accurate. The least-squares fit becomes unstable when the $m_2(-t)^{\Delta_2}$ term is included in the analysis. This applies for $\Delta_2 = 2\Delta_1$ as well as for $\Delta_2 = 0.9$ (Rehr 1979).

4. Discussion

The energy data analysis, which includes a confluent singularity, leads to an estimate for A^+/A^- in accordance with the universal value. This result differs from the findings of a similar analysis of the $S=\frac{1}{2}$ Ising ferromagnet (Knak Jensen and Mouritsen 1982), where accordance was obtained only in the absence of a confluent singularity. The origin of the difference is not clear. It has been suggested (Adler 1983) that the estimate used for T_c in the $S=\frac{1}{2}$ case will favour the absence of a confluent singularity. The argument is that T_c is derived from a series analysis, which neglects confluent singularities. It may therefore be expected that use of these critical temperatures may—in a self-consistent way—result in least-squares analyses yielding a zero amplitude for the confluent singularity. The point is well taken and Adler proceeds to calculate T_c with a method allowing for a confluent singularity. The relative difference between the two sets of estimates for T_c is at the very most 4×10^{-4} for the $S=\frac{1}{2}$ Ising ferromagnet arrayed on a simple cubic lattice. The new critical temperatures have been used in an analysis of the energy data. The derived estimate for A^+/A^- does not accord with the universal value. The situation might have been different had the data been closer to $t=0$ than 6×10^{-3}.

The argument of Adler is applicable also in the present case of the $S=\infty$ Ising ferromagnet as T_c is derived from a procedure, which neglects confluent singularities. However, in this case the estimate for A^+/A^- accords with the universal value.

The data analysis reported here does not lead to agreement of D^+/D^- with the expected theoretical value. The reason is probably that the estimates for D^+ and D^- contain significant contributions from higher-order correction terms. These are difficult to separate unless the statistical errors become much smaller.

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Note added in proof. Recently, and interesting analysis has been performed on Nickel's 21st-order series for the susceptibility and correlation length for the spin-S Ising ferromagnet arrayed on a BCC lattice (Ferer M and Velgakis M J 1983 *Phys. Rev.* B **27** 2839–54). The authors use an unbiased method of confluent singularity analysis tailored to the loose-packed lattices. Ferer and Velgakis find that 'the confluent correction is apparently not significant for spin-$\frac{1}{2}$'. Furthermore, the amplitude of the confluent singularity is finite for $S=\infty$. These findings are in accordance with the present investigation of the heat capacity of the $S=\infty$ Ising ferromagnet on a simple cubic lattice and the previous investigation of the same function in the $S=\frac{1}{2}$ case (Knak Jensen and Mouritsen 1982).

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