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LETTER TO THE EDITOR

Correction to the leading singularity of the order parameter of the four-dimensional Ising ferromagnet

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Abstract. The Monte Carlo technique is used to calculate the order parameter, Φ, of the four-dimensional spin-$\frac{1}{2}$ Ising ferromagnet in a simple hypercubic lattice. The order-parameter data are described by $\Phi(t)=B(-t)^{1/2}|\ln(-t)|^{1/3}[1+Q\ \ln|\ln(-t)|/|\ln(-t)|]$ in the range $0{\cdot}01\leqslant -t\equiv(T_c-T)/T_c<0{\cdot}56$ with parameters $B=1{\cdot}543\pm0{\cdot}002$ and $Q=-0{\cdot}030\pm0{\cdot}02$. The form of $\Phi(t)$ agrees with that predicted by renormalisation group theory.

Much research is currently being carried out in order to test renormalisation group (RG) predictions of critical behaviour using independent theoretical approaches and experimental measurements. Investigations of four-dimensional systems are of special importance in this context because exact solutions to the RG equations may be obtained in the case of four dimensions.

In this Letter we are concerned with the four-dimensional Ising model for which Sykes (1979) has recently extended various high- and low-temperature series expansions. Gaunt *et al* (1979) have analysed the high-temperature series for the susceptibility and for the fourth field derivative of the free energy, and found that the form of the critical singularities is in agreement with the RG theory. Furthermore, McKenzie *et al* (1979) have shown that the asymptotic behaviour of the series for the critical isotherm is consistent with the RG prediction.

The RG theory predicts that the thermodynamic singularities for four-dimensional systems are given by mean-field power laws multiplied by a fractional power of a logarithm (Brézin *et al* 1973, Wegner and Riedel 1973). For example, the leading singularity of the order parameter of the Ising model is predicted to be (Larkin and Khmel'nitskii 1969)

$$\Phi(t)\propto(-t)^{1/2}|\ln(-t)|^{1/3} \qquad \text{with } t\equiv(T-T_c)/T_c<0, \tag{1}$$

where T_c is the critical temperature. Measurements on uniaxial ferromagnets with long-range interactions, which in the limit $|t|\to 0$ are expected to have the same singularities as the four-dimensional Ising ferromagnet, agree with (1) (Brinkman *et al* 1978, Griffin *et al* 1977, Kötzler and Eiselt 1976, Frowein and Kötzler 1976). Furthermore, we have recently probed the validity of (1) by a Monte Carlo (MC) calculation of $\Phi(t)$ for the four-dimensional spin-$\frac{1}{2}$ Ising ferromagnet in a simple hypercubic lattice (Mouritsen and Knak Jensen 1979). The MC data, $\Phi^{MC}(t)$, agree with (1) for $0{\cdot}01\leqslant -t<0{\cdot}4$ and determine the critical amplitude, B, pertaining to Φ when $1{\cdot}53<B<1{\cdot}56$. All this evidence suggests that (1) is well established.

A more comprehensive investigation of the RG predictions is to study the correction terms to the leading singularity (1). The forms of such correction terms are known above T_c for the susceptibility and the heat capacity (Brézin and Zinn-Justin 1976), although no experimental observations have as yet been published. Below T_c the first-order correction is expected to modify (1) as (Brézin *et al* 1976)

$$\Phi(t) = B(-t)^{1/2}|\ln(-t)|^{1/3}[1 + Q \ln|\ln(-t)|/|\ln(-t)|], \tag{2}$$

where Q is a constant.

We have extended our MC study to obtain high-precision data for Φ in the t region where our previous data did not fit (1), i.e. $-t > 0{\cdot}4$. The calculations are performed on a 12^4 spin system subjected to toroidal periodic boundary conditions. A conventional MC importance sampling technique (Binder 1979) is employed, and the raw computer data are analysed using coarse graining techniques (Mouritsen and Knak Jensen 1978). At each temperature the calculations are repeated for several different initial configurations in order to obtain data with a typical uncertainty of Φ as low as 2×10^{-4}. Trial calculations on smaller lattices demonstrate that finite-size effects are unimportant for $-t \geqslant 0{\cdot}01$.

The new MC data, as well as the data previously reported, are analysed in terms of equation (2) using the most recent estimate of the critical temperature, $T_c = (6{\cdot}6817 \pm 0{\cdot}0015)J/k_B$, where J is the nearest-neighbour exchange parameter (Gaunt *et al* 1979). This estimate is obtained from an analysis of the higher-temperature series expansion of the susceptibility, assuming a mean-field singularity modified by a logarithmic factor. The agreement between T_c and the critical temperature estimated from the MC calculations is discussed by Mouritsen and Knak Jensen (1979).

The MC data are analysed by a least-squares fitting minimising the weighted sum

$$\sigma(B, Q) = \sum_{t \in S_t} [\![\{\Phi^{MC}(t) - B(-t)^{1/2}|\ln(-t)|^{1/3}[1 + Q \ln|\ln(-t)|/|\ln(-t)|]\}/\Delta\Phi^{MC}(t)]\!]^2. \tag{3}$$

In equation (3), $\Delta\Phi^{MC}(t)$ is the uncertainty of $\Phi^{MC}(t)$, and S_t specifies the interval $\{t|0{\cdot}01 < -t < t_{max}\}$, where t_{max} denotes a cut-off value of the reduced temperature. The function $\sigma(B, Q)$ is calculated for various values of t_{max}. We find for $t_{max} \approx 0{\cdot}4$, which corresponds to the interval previously investigated without the correction term, that inclusion of the correction term gives an improved fit with $-0{\cdot}02 < Q < -0{\cdot}03$ and the central value of B unchanged. For larger values of t_{max} ($\leqslant 0{\cdot}56$) the best fit is obtained for the same central B-value and for $Q \simeq -0{\cdot}03$. For $t_{max} \geqslant 0{\cdot}56$ the minimum value of σ starts to increase. In the interval $S_t = \{t|0{\cdot}01 < -t < 0{\cdot}56\}$, the function $\sigma(B, Q)$ is found to have a pronounced global minimum close to the point $(B, Q) = (1{\cdot}543, -0{\cdot}030)$. The variation of $\sigma(B, Q)$ in the neighbourhood of this point is shown in figure 1, which demonstrates that the overall quality of the data fitting is very sensitive to B and Q.

The result of our data analysis is

$$B = 1{\cdot}543 \pm 0{\cdot}002 \qquad \text{and} \qquad Q = -0{\cdot}030 \pm 0{\cdot}002, \tag{4}$$

where the uncertainties of both T_c and Φ^{MC} have been taken into account in estimating the error limits. We note that the value of B determined in this way is consistent with the previously reported value which was derived by setting $Q = 0$. However, when the correction term is taken into account the estimated uncertainty of B is reduced by almost a factor of ten.

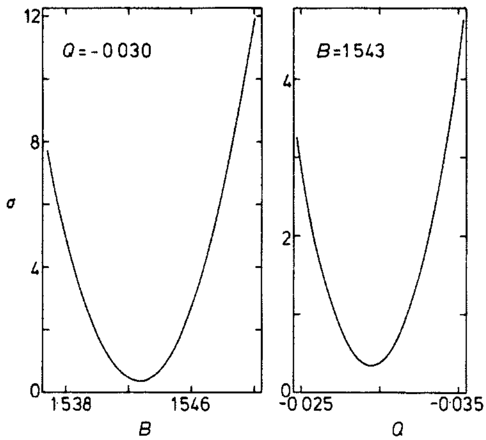

Figure 1. Plot of $\sigma(B, Q = -0\cdot030)$ and $\sigma(B = 1\cdot543, Q)$ against B and Q respectively. σ is defined in equation (3) and gives, for the reduced temperature interval $S_t = \{t|0\cdot01 < -t < 0\cdot56\}$, a measure of the overall quadratic deviation between the Monte Carlo data for the order parameter and the fitting function $B(-t)^{1/2}|\ln(-t)|^{1/3}[1 + Q \ln|\ln(-t)|/|\ln(-t)|]$. The ordinates are given in a common arbitrary unit.

In figure 2 we show $\Phi(t)$ calculated from equations (2) and (4) together with Φ^{MC}. Figure 2 only contains data for $-t \geqslant 0\cdot3$, because the smallness of Q makes the inclusion of the correction term most noticeable at relatively high values of $|t|$. The low-temperature series expansion for Φ to order $[\exp(-4J/k_BT)]^{35}$ (Sykes 1979)

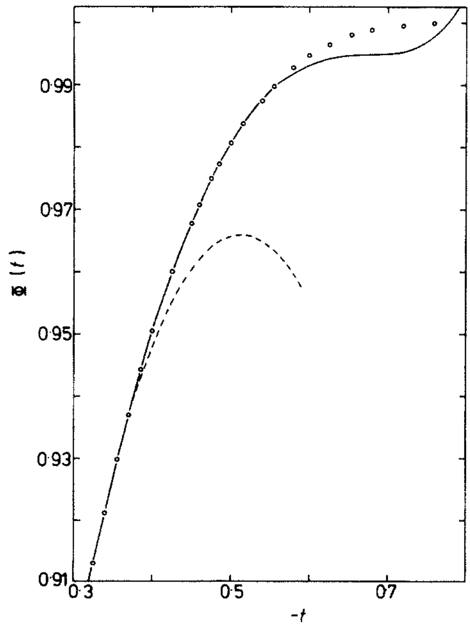

Figure 2. Temperature variation of the order parameter of the four-dimensional spin-$\frac{1}{2}$ Ising ferromagnet in a simple hypercubic lattice. O: Monte Carlo data; full line: $\Phi(t) = 1\cdot543(-t)^{1/2}|\ln(-t)|^{1/3}[1 - 0\cdot030 \ln|\ln(-t)|/|\ln(-t)|]$; dashed line: $\Phi(t) = 1\cdot543(-t)^{1/2}|\ln(-t)|^{1/3}$.

reproduces the MC data within the uncertainty for $-t \geqslant 0 \cdot 46$ which corresponds to $\Phi(t) \geqslant 0 \cdot 97$.

In conclusion, we have used the Monte Carlo technique to obtain data for the order parameter of the four-dimensional Ising ferromagnet. These data allow a comparison with the theoretical expected expression which includes a correction term to the leading singularity. We find that this expression provides a better fit to our data over a wider range of reduced temperatures than the uncorrected expression. In addition, we have obtained the value of the coefficient pertaining to the correction term. This value may also be calculated theoretically using the renormalisation group. We suggest such a calculation to serve as an assessment of the renormalisation group approach.

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