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LETTER TO THE EDITOR

Spin density correlation functions below the critical point

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Abstract. Low-temperature expansions for the second moment of the spin density correlation function have been developed for a generalized Ising model which includes three- and four-body interactions. The evidence for a downward shift in the value of $\gamma' + 2\nu'$ for a three-dimensional pure triplet Ising model, which was previously predicted by the thermodynamic functions and scaling theory, is well confirmed.

The nature of the spin density correlation functions

$$\Gamma(\boldsymbol{r}, T, H) = \langle (s(\boldsymbol{0}) - \langle s(\boldsymbol{0})\rangle)(s(\boldsymbol{r}) - \langle s(\boldsymbol{r})\rangle)\rangle \tag{1}$$

in Ising and Heisenberg model assemblies has been well studied in the zero-field ($H = 0$) and high-temperature ($T \geqslant T_c$) domain (Fisher and Burford 1967, Jasnow and Wortis 1972, Ferrer and Wortis 1972, Ritchie and Fisher 1972, Moore *et al* 1969). At the present time the only corresponding calculations in the low-temperature domain ($T \leqslant T_c$) are those of Tarko and Fisher (1973). These authors obtained low-temperature and general field expansions for the moments of the spin density correlation function

$$\mu_t(H, T) = \sum_{\boldsymbol{r}} \left|\frac{\boldsymbol{r}}{a}\right|^t \Gamma(\boldsymbol{r}, T, H) \tag{2}$$

of the nearest-neighbour Ising model on the BCC, SC and SQ lattices. It is expected that the moment functions diverge at the critical temperature according to the asymptotic form

$$\mu_t \sim \begin{cases} (T_c - T)^{-(\gamma' + t\nu')} & T \to T_c^-, \quad H = 0 \quad (3) \\ (T - T_c)^{-(\gamma + t\nu)} & T \to T_c^+, \quad H = 0. \quad (4) \end{cases}$$

Thus on the assumption that $\gamma = \gamma' = \frac{5}{4}$ for the three-dimensional Ising model Tarko and Fisher obtained the first *direct* estimate of the low-temperature exponent of the coherence length, and found that $2\nu' = 1{\cdot}28 \pm 0{\cdot}04$ (SC lattice) which in view of the earlier estimate $2\nu = 1{\cdot}282 \pm 0{\cdot}005$ (Fisher and Burford 1967, Moore *et al* 1969) is a result which is consistent with the scaling prediction $\nu = \nu'$.

The purpose of this letter is to report a calculation of the low-temperature expansion of μ_2 for a generalized Ising model which includes three- and four-body interactions. This model, which has been studied previously (Wood and Griffiths 1974) in relation to the thermodynamic functions, is defined on the FCC lattice with a Hamiltonian

$$\mathscr{H} = -J_2 \sum_{\mathrm{nn}} \sigma_i\sigma_j - J_3 \sum_{ijk} \sigma_i\sigma_j\sigma_k - J_4 \sum_{ijkl} \sigma_i\sigma_j\sigma_k\sigma_l - mH \sum_{i=1}^{N} \sigma_i, \tag{5}$$

where the interaction terms are over nearest-neighbour (nn) lines, triangles and tetrahedra.

For such models the direct technique of developing the expansions of $\mu_t(T, H)$ can be substantially aided by an extension of the simplex transformation (Wood and Griffiths 1973) which has been developed previously for expanding the free energy. The key relation in this formulation of μ_t is a modification of equations (16) and (23) given by Wood and Griffiths (1973) which takes the form

$$\mu_t(\mu, u_1, u_2, \ldots, u_{n-1}) = \sum_{s=2}^{\infty} g_s^{(t)}(u_1, u_2, \ldots, u_{n-1})\mu^s \tag{6}$$

$$= \sum_{n_{s_j}\, j\in J\cup K} \Phi_{\{n_{s_j}, j\in J\cup K\}}(\mu) \prod_{i\in K}(1-u_{i-1})^{n_{s_i}} \prod_{i\in J} v_{j-1}^{n_{s_j}} \Big/ (1+\mu)^{\Sigma_{j\in J\cup K} jn_{s_j}+2} \tag{7}$$

where $\Phi_{\{n_{s_j}, j\in J\cup K\}}(\mu)$ are a new class of antisymmetric or symmetric high-temperature polynomials relating to the moment expansions.

A number of complete high-field polynomials $g_s^{(t)}$ $(t = 2, 4)$ have been determined for several models of the type (5); these numerical data and further details of the methodology will be given elsewhere. Here we report upon the direct estimation of $\gamma' + 2\nu'$ for the pure triplet case $J_2 = J_4 = 0$ in (5), denoted by $\{0, 1, 0\}$. On the previously assumed phase boundary ($H = 0$, $T \leqslant T_c$)† we obtain

$$\mu_2(0, T) = 48u^{10} - 48u^{12} + 192u^{13} + 1632u^{14} - 2304u^{16} + 9600u^{17} + 38400u^{18}$$
$$+ 768u^{19} - 71472u^{20} + 284928u^{21} + 890304u^{22} + \ldots . \tag{8}$$

Previous studies of the exponents α, β and δ (Wood and Griffiths 1974) have strongly supported the validity of the scaling relations for this $\{0, 1, 0\}$ model, and have yielded quite unusually convergent estimates of a critical point $u_c = \exp(-8J_3/kT_c)$, which support the conjecture that $u_c = \frac{1}{2}$. Although the moment series (8) is much less well behaved than the previous series, the presence of a singularity at $u_c \simeq \frac{1}{2}$ is again confirmed; typical examples of high-order Padé approximants (unbiased) yield $u_c = 0{\cdot}4970$, 0·4966, 0·5080 and 0·5058. A scatter diagram of these unbiased estimates is shown in figure 1, where estimates of u_c are plotted against the corresponding estimates of the combined exponent $\gamma' + 2\nu'$. The corresponding analysis for the pure pair model $\{1, 0, 0\}$ is shown for comparison.

The previous estimates of α, β and δ when combined with the scaling relations predict a value $2\nu' + \gamma' = 2{\cdot}14 \pm 0{\cdot}01$ for the $\{0, 1, 0\}$ case, which is a significant shift from the value $2\nu' + \gamma' = 2{\cdot}53$ obtained on similar assumptions for the conventional case $\{1, 0, 0\}$. A shift of this size should be evidenced using the usual methods of series analysis. On the assumption that $u_c = \frac{1}{2}$ for $\{0, 1, 0\}$ and that $u_c = \exp(-4J_2/kT_c) = 0{\cdot}6647$ (Sykes *et al* 1972) for $\{1, 0, 0\}$, figure 1 indicates that the values $2{\cdot}42 \pm 0{\cdot}02$ and $2{\cdot}27 \pm 0{\cdot}01$ of $2\nu' + \gamma'$ for $\{1, 0, 0\}$ and $\{0, 1, 0\}$ respectively would be obtained in approximants having accurate roots (u_c) at the available orders.

Additional evidence on the value of $2\nu' + \gamma'$ can be obtained from the biased approximants to $(u - u_c)\, \mathrm{d}\ln(\mu_2)/\mathrm{d}u$. A typical sequence of $[n, n+j]$ approximants for the

† Watts and Enting (1975) have conjectured that there is no phase transition at $H = 0$ for this model. On the basis of their observation intuition certainly suggests that the magnetization will go to zero at sufficiently high temperatures in a negative field, and therefore one might expect a transition line terminating at a point H_c, T_c. Our analysis possibly suggests that H_c is small and that the line $H = 0$ is sufficiently close to H_c for the numerical analysis to reflect the essential features of the critical point.

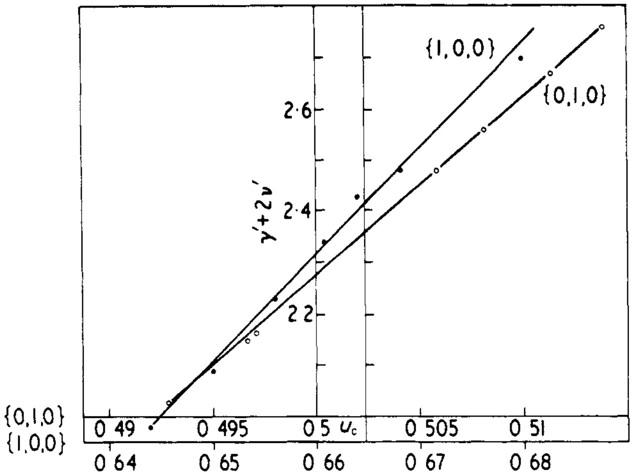

Figure 1. A scatter diagram which plots the estimates of u_c against the estimates of the combined exponent $2\nu'+\gamma'$ obtained from the Padé approximants to the logarithmic derivative of μ_2. The results for the pure pair Ising model are included for comparison.

$\{1,0,0\}$ model is the $n = 6$ row, which yields

$$\begin{array}{lcccccc} j & = 4 & 5 & 6 & 7 & 8 & 9 \\ 2\nu'+\gamma' & = 2{\cdot}41 & 2{\cdot}42 & 2{\cdot}44 & 2{\cdot}44 & 2{\cdot}46 & 2{\cdot}47 \end{array} \qquad (u_c = 0{\cdot}6647) \tag{9}$$

and for the $\{0,1,0\}$ model the $n = 4$ and 5 rows are respectively

$$\begin{array}{lcccc} j & = 4 & 5 & 6 & 7 \\ 2\nu'+\gamma' & = 2{\cdot}36 & 2{\cdot}34 & 2{\cdot}26 & 2{\cdot}27 \end{array} \tag{10}$$

$$\begin{array}{lcccc} j & = 3 & 4 & 5 & 6 \\ 2\nu'+\gamma' & = 3{\cdot}85 & 2{\cdot}34 & 2{\cdot}36 & 2{\cdot}27 \end{array} \qquad (u_c = \tfrac{1}{2}). \tag{11}$$

Thus the $\{1,0,0\}$ values appear to be converging from below; in summary of the overall results we find $2\nu'+\gamma' = 2{\cdot}50 \pm 0{\cdot}05$, and assuming $\gamma' = \frac{5}{4}$ this yields $2\nu' = 1{\cdot}25 \pm 0{\cdot}05$, which confirms the estimates of Tarko and Fisher (1973). In sequences such as (10) and (11) the evidence for a downward shift in $2\nu'+\gamma'$ is very definite; these sequences seem to be converging from above. The scatter diagram for the $\{1,0,0\}$ points, when combined with the probable result $2\nu'+\gamma' = 2{\cdot}53$ (using the high-temperature estimates), indicates a truncation error of $0{\cdot}11 \pm 0{\cdot}02$. Allowing for the decreasing trend in sequences such as (10) and (11), we think that the result

$$\gamma'+2\nu' = 2{\cdot}20 \pm 0{\cdot}06 \qquad \{0,1,0\} \text{ model} \tag{12}$$

summarizes this numerical study, and that the overall results are consistent with the earlier predictions using scaling theory (Wood and Griffiths 1974).

Note added in proof. A comprehensive series expansion study of $\Gamma(\boldsymbol{r}, T, H)$ for the FCC $\{1,0,0\}$ model has recently been given by Ritchie and Essam (1975).

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