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LETTER TO THE EDITOR

Exponents far from T_c for ferromagnets with second-neighbour interactions and for the Baxter–Wu model

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Abstract. The temperature dependence of the paramagnetic zero-field susceptibility χ is calculated for the second-neighbour $S = \frac{1}{2}$ Heisenberg model and for the Baxter–Wu model, from Padé approximants to existing high-temperature series expansions and by Monte Carlo simulations. The data are well represented by a power law $\chi T = (t')^{-\gamma}$ using the critical susceptibility exponent γ over the whole paramagnetic temperature range when a non-linear scaling variable t' is used; namely $t' = 1 - T_c/T$ for the second-neighbour models and $t' = 1 - (T_c/T)^2$ for the Baxter–Wu model.

In a series of recent publications (de Jongh *et al* 1970, Souletie and Tholence 1983, Fähnle and Souletie 1984, 1985, 1986, Arrott 1984, 1985, Carré *et al* 1986), the paramagnetic susceptibilities χ of many spin systems have been analysed using the non-linear variable $t' = (T - T_c)/T_c$. It has been shown that χ may be described to a high degree of accuracy by a power law (generalised Curie–Weiss law) of the form

$$\chi T = (t')^{-\gamma} \qquad t' = (T - T_c)/T \tag{1}$$

not only in the critical regime (γ is the asymptotic critical susceptibility exponent), but sometimes up to infinitely high temperatures (all temperatures are in units of J/k_B). To test the validity of equation (1), a temperature dependent exponent

$$\hat{\gamma}(T) = -\partial \ln(\chi T)/\partial \ln t' \tag{2}$$

has been introduced that is by definition equal to γ if equation (1) holds. In some special cases the quantity $\hat{\gamma}(T)$ is nearly temperature independent up to infinitely high temperatures (see below).

Equation (1) may be conceived of as an interpolation formula between the critical behaviour at T_c (including the analytic corrections due to the use of the non-linear variable t' (Fisher 1983)) and the very high-temperature behaviour that, up to the first correction term, reads

$$\chi T = 1 + a/T. \tag{3}$$

Here the quantity a is the coefficient of the first-order term in the high-temperature series, and from equation (2) we obtain

$$\hat{\gamma}(T \to \infty) =: \hat{\gamma}(\infty) = a/T_c. \tag{4}$$

Comparing equation (3) with the high-temperature expansion of equation (1) it becomes obvious that the generalised Curie–Weiss law may be a useful interpolation formula if

$\hat{\gamma}(\infty) = a/T_c \simeq \gamma$. Equation (1) is exactly valid in the mean-field limit, i.e. for coordination number $q = \infty$, for which we have $\hat{\gamma}(\infty) = \gamma = 1$. For finite q, the quantity $\hat{\gamma}(\infty) \neq 1$ is in general different from the asymptotic critical value γ. This holds even for dimensions $d \geqslant 4$ for which γ attains its mean-field value of 1, whereas, for instance, for the hypercubical Ising model an expansion (Fisher and Gaunt 1964) up to the first order of $1/q = 1/2d$ yields $\hat{\gamma}(\infty) = a/T_c = 1 + 1/2d$. For $d = 3$, the generalised Curie–Weiss law holds very well for the Ising and the $S = 1$ Heisenberg models on a body-centred cubic (BCC) and face-centred cubic (FCC) lattice (cf figures 1 and 2 of Fähnle and Souletie 1984). For instance, for the BCC Ising model the Padé approximant of Baker (1961) yields $\hat{\gamma}(\infty) = 1.259$ and $\gamma = 1.25$. For $d = 2$, equation (1) is best fulfilled for the square Ising model (figure 1 of Fähnle and Souletie 1984).

In the present letter it is argued that the validity of the generalised Curie–Weiss law, equation (1), may be considerably improved for some Ising and $S = \frac{1}{2}$ Heisenberg models when considering second-neighbour interactions. Furthermore, we propose a modified version of the generalised Curie–Weiss law for the Baxter–Wu model on a triangular lattice, for which the susceptibility cannot be described by equation (1) since the first term in the high-temperature expansion of this model (Wood and Griffiths 1973) is quadratic in $1/T$.

We will now consider a model of a ferromagnet with second-neighbour interactions. This model is defined by the Hamiltonian

$$H = -\tfrac{1}{2}J_1 \left(\sum_{\mathrm{NN}} \sigma_i \sigma_j + \alpha \sum_{\mathrm{SN}} \sigma_k \sigma_m \right) \tag{5}$$

where the first sum runs over all nearest-neighbour spins (NN) and the second sum over all second-neighbour spins (SN), and $\alpha = J_2/J_1$ denotes the ratio of the corresponding exchange integrals. Power series expansions for χT for various α have been obtained for the $S = \frac{1}{2}$ Heisenberg model and for the Ising model by Dalton and Wood (1965, 1969), for instance for the simple cubic (SC), BCC and FCC lattices.

We first outline our general idea for the case of Ising models. When considering only nearest-neighbour interactions ($\alpha = 0$), the value for $\hat{\gamma}(\infty)$ is slightly smaller (larger) than the value of γ for the FCC (SC) lattice (figure 1 of Fähnle and Souletie 1984). This may be corrected by switching on the second-neighbour interactions. According to Dalton and Wood (1969), the critical temperature as a function of α may be written as $T_c(\alpha) = T_c(0)(1 + m_1\alpha)$ for $0 \leqslant \alpha \leqslant 1$, with $m_1 = 0.61$ (2.47) for the FCC (SC) lattice. Since the coefficient of the first-order term in the high-temperature series is given by $a(\alpha) = a(0)(1 + \alpha)$, equation (4) yields

$$\hat{\gamma}(\infty, \alpha) = \hat{\gamma}(\infty, 0)[(1 + \alpha)/(1 + m_1\alpha)]. \tag{6}$$

Increasing α we arrive at larger (smaller) values of $\hat{\gamma}(\infty, \alpha)$, and for a certain value of α the high-temperature exponent $\hat{\gamma}(\infty, \alpha)$ is equal to the asymptotic critical value γ. We would then expect (1) to hold rather accurately over the whole paramagnetic regime.

The improvements that may be achieved by inserting a non-zero value of α are much greater for the $S = \frac{1}{2}$ Heisenberg models, for which the $\hat{\gamma}(\infty, 0)$ values differ rather drastically from γ (cf. figure 1 of Fähnle and Souletie 1984). To demonstrate this we have constructed from the high-temperature series expansions of Dalton and Wood (1965) the [2, 3] and [3, 2] Padé approximants to the series $(\chi T)^{3/4}$. This fixes the asymptotic critical value at $\gamma = \frac{4}{3}$, which corresponds to the estimates of γ on the basis of these series expansions (Dalton and Wood 1965). The [2, 3] and [3, 2] approximants yield slightly different results for $\alpha = 0$, but for $\alpha \geqslant 0.1$ these differences are negligibly small. We therefore only exhibit the results from the [2, 3] approximants. It should be

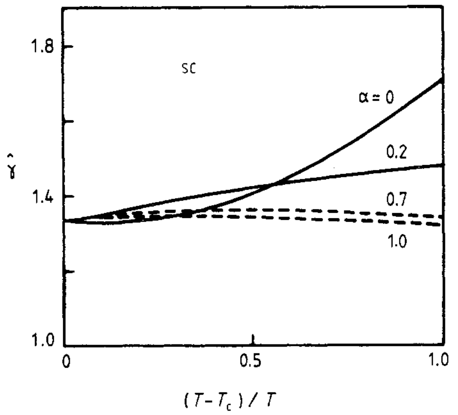

Figure 1. $\hat{\gamma}(T)$ for the SC $S=\frac{1}{2}$ Heisenberg model with various values of α.

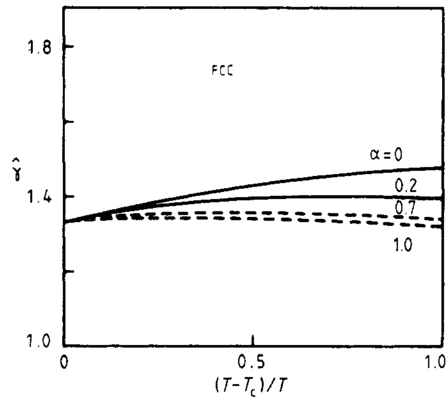

Figure 2. $\hat{\gamma}(T)$ for the FCC $S=\frac{1}{2}$ Heisenberg model with various values of α.

noted that the values of γ and of $\hat{\gamma}(\infty, 0)$ are not exactly the same as those given in figure 2 of Fähnle and Souletie (1984), because in the latter paper the calculations were based on the series expansions of Ritchie and Fisher (1972), which include more terms than those of Dalton and Wood (1965). However, our main point, namely that it appears possible that the simple exponent law (1) holds far from T_c, does not depend that much for instance on the accuracy of γ: if we had a series expansion up to the same order as the one of Ritchie and Fisher (1972), also for non-zero values of α, an analysis on the present line would certainly produce the same general result.

From figures 1 and 2 it becomes obvious that the validity of the generalised Curie–Weiss law (1) may indeed be considerably improved over the whole paramagnetic regime (note that $(T-T_c)/T = 1$ corresponds to infinitely high temperatures!) by taking into account second-neighbour interactions. For certain values of $\alpha \neq 1$ a perfect agreement between $\hat{\gamma}(\infty)$ and γ is obtained, but the smallest overall deviations of $\hat{\gamma}(T)$ from γ are found for α-values of about 1.

The Baxter–Wu model is in Ising model defined on a triangular lattice with the Hamiltonian

$$H = -J\sum \sigma_i\sigma_j\sigma_k \tag{7}$$

where the sum runs over all triangles made up of nearest-neighbour spins. In Fähnle and Souletie (1986) it has been noted that the generalised Curie–Weiss law (1) does not hold for this model, because the first term in the series expansion (Wood and Griffiths 1973)

$$\chi T = 1 + 6v^2 + 30v^4 + 180v^6 + \ldots \tag{8}$$

$$v = \tanh(1/T) \tag{9}$$

is quadratic rather than linear in $1/T$. We now suggest a modified version of the generalised Curie–Weiss law of the form

$$\chi T = (t')^{-\gamma} \qquad t' = 1-(T_c/T)^2. \tag{10}$$

To test the validity of equation (10) we again consider the exponent $\hat{\gamma}(T)$ defined by (2), yielding with equations (8, 9) the high-temperature exponent $\hat{\gamma}(\infty) = 6/T_c^2$. With the exact result $T_c = 2/(\ln\sqrt{2}+1)$, this gives $\hat{\gamma}(\infty) = 1.16523$, which compares excellently to the asymptotic exponent value $\gamma = 7/6 \simeq 1.16666$ (Baxter 1982).

Since the series (8) is rather short it does not make sense to test for the overall validity of (10) by constructing the Padé approximants. Instead, we have performed Monte

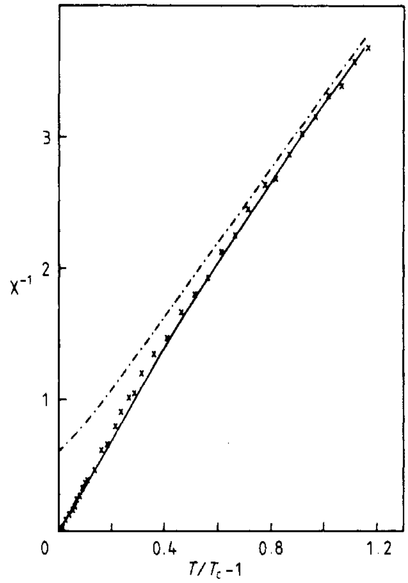

Figure 3. Temperature dependence of χ for the Baxter–Wu model. Full curve: generalised Curie–Weiss law, equation (10), with $\gamma = \frac{7}{6}$; chain curve: high-temperature series, equation (8); crosses: Monte Carlo data.

Carlo simulations on the line described by Novotny and Landau (1981) (48 × 48 lattice with periodic boundary conditions, four independent runs for each temperature, 8000 Monte Carlo spin-flip trials per spin for each run, the first 2650 omitted from thermal averages). Figure 3 shows that the Monte Carlo data are excellently described by the modified version of the generalised Curie–Weiss law (10) over the whole paramagnetic temperature range (the small deviations at $(T - T_c)/T_c \simeq 0.3$–0.4 possibly do not have a physical meaning but may result from uncertainties in the Monte Carlo data due to very large thermal fluctuations in this system; cf. Novotny and Landau 1981).

To conclude, we have discussed some more systems for which the paramagnetic zero-field susceptibility may be well described for all temperatures by a power law $\chi T = (t')^{-\gamma}$ using the asymptotic critical exponent γ when a proper non-linear variable t' is used instead of the linear variable $(T - T_c)/T_c$.

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