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LETTER TO THE EDITOR

Transformation analysis of the Heisenberg model susceptibility series

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Abstract. We have applied a systematic method for series transformation to the susceptibility of the Heisenberg model on various cubic lattices. The resulting series are sufficiently smooth for extrapolation by means of Neville tables, and we conclude that the exponent γ has the value $1\cdot40\pm0\cdot02$ for both the quantum spin-$\frac{1}{2}$ and classical models.

During the past fourteen years the Heisenberg model of ferromagnetism has been extensively studied by series expansion techniques. (For a definition of the model see the review by Rushbrooke *et al* 1974.) However, none of the critical exponents is yet known with high precision: for example the more recent estimates of the zero field susceptibility exponent γ range from $1\cdot36\pm0\cdot04$ up to around $1\cdot43$, and the question of its spin dependence still remains unresolved. The main reasons for this are the shortness of the series (the later coefficients are extremely difficult to calculate) and the location of non-physical singularities in the complex plane of the expansion variable.

Most of the exponent estimates to date have been based on Padé analysis (e.g. Baker *et al* 1967, Ritchie and Fisher 1972), on the graphical extrapolation of ratio plots (Lee and Stanley 1971), or most recently on confluent singularity analysis (Camp and Van Dyke 1976). However, the analysis method which arguably makes least assumption as to the form of the critical singularity—the numerical extrapolation of smooth ratio sequences—has been applied only to the classical (infinite spin) model on the FCC lattice, by Ferer *et al* (1971). These authors used the Neville table method (see for example Gaunt and Guttmann 1974) to extrapolate ratios and sequences obtained by 'critical point renormalization', with the conclusion $\gamma=1\cdot405\pm0\cdot020$. For spin-$\frac{1}{2}$ and for other lattices the presence of non-physical singularities near to or inside the so called 'physical disc' causes irregularities in the sequences involved, and prevents the direct use of this type of extrapolation.

By employing a systematic method for choosing transformations (Pearce 1975) we have obtained, for the spin-$\frac{1}{2}$ and classical models on all cubic lattices, new susceptibility series which are sufficiently smooth for extrapolation by means of Neville tables, in most cases up to the fourth or fifth order. The smooth behaviour results from the transformed function having all its nearer singularities to the origin on the positive real axis, principally at u_c say (corresponding to the physical singularity) and at u_1 where

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$u_1 \gtrsim 1{\cdot}2u_c$. If r_n are the ratios of successive coefficients of the transformed series, we then have from the theorems of Darboux (1878):

$$r_n \sim \frac{1}{u_c}\left(1+\frac{\gamma-1}{n}+\frac{b}{n^2}+\mathrm{O}\left(\frac{1}{n^3}\right)\right)+c\left(\frac{u_c}{u_1}\right)^n \tag{1}$$

where b and c are constants which, together with u_c, depend on the transformation employed. In all cases studied it was found, by the use of a 'mimic' function, that the term in $(u_c/u_1)^n$ which vanishes exponentially fast as $1/n$ tends to zero gave a contribution to the Neville entries which was smaller than the general scatter. The term b/n^2 was however appreciable in some cases, and in these it was necessary to go to the second order to obtain reasonable convergence.

Thus to estimate the value of the critical point and exponent, a Neville table was calculated for the ratios and this was used to obtain an 'unbiased' value (in the sense of Hunter and Baker 1973) for the singularity location, u_c, and its uncertainty. This u_c range was then employed in calculating a corresponding γ range by means of further Neville and Padé tables. As pointed out by Rushbrooke *et al* (1974), the value chosen for the critical temperature is crucial in determining the value of the exponent. In the present estimates, the γ range quoted corresponds to what we consider to be the full u_c range consistent with the available series.

Since the procedure was essentially the same for all the series analysed, we describe it for one case only and merely state the final results for the others. The series chosen is that for the spin-$\frac{1}{2}$ model on the SC lattice: this appears to be the one most seriously influenced by non-physical singularities (Lee and Stanley 1971). Padé analysis indicates singularities in the K-plane (where $K=J/kT$ is the expansion variable) at approximately $0{\cdot}6$ (the physical singularity), $-0{\cdot}08 \pm 0{\cdot}50\mathrm{i} \pm (0{\cdot}01 \pm 0{\cdot}01\mathrm{i})$, and possibly $-0{\cdot}7$. Thus the circle of convergence appears to be determined by the pair of singularities in the left half-plane, rather than by the physical singularity.

For this particular distribution of singularities, the use of the systematic method referred to above leads to the following transformation: the susceptibility $\chi(K)$ is transformed to a new function $\tilde{\chi}(v)$, with v related to K by

$$v = u/(1+u/0{\cdot}7)$$

where

$$u = K/[(1-K/a)(1-K/a^*)]^{1/2},$$

in which $a = 0{\cdot}08+0{\cdot}50\mathrm{i}$. This transformation leaves the exponent of the critical singularity invariant, and is designed to result in a singularity distribution of the kind described earlier. That this was actually achieved was verified on Padé analysis of the series for $\tilde{\chi}(v)$, which indicated singularities in the v-plane only near $v = 0{\cdot}24$ (corresponding to the physical singularity), $0{\cdot}29$, $0{\cdot}42$ and $-1{\cdot}33$. As intended, the ratios of the transformed coefficients formed the required smooth sequence, suitable for Neville table extrapolation to find the value of v_c. Such a table was constructed and showed convergence within the scatter by the second order, the majority of the entries in the second to fourth orders lying within the range $4{\cdot}220 \pm 0{\cdot}005$, and the remainder close to this. We take this range as our estimate for the ratio extrapolant v_c^{-1}, corresponding to $v_c = 0{\cdot}2370 \pm 0{\cdot}0003$, or $K_c = 0{\cdot}5942 \pm 0{\cdot}0020$.

The central v_c value was then used in calculating the sequence of exponent estimates γ_n based on (1):

$$\gamma_n = 1 + n(r_n v_c - 1) = \gamma + b/n + \mathrm{O}(1/n^2). \tag{2}$$

A Neville table for this sequence (reproduced in table 1) shows approximate convergence to a γ value by the first order, as expected from the behaviour of the ratios. To provide an additional estimate for the exponent, Padé approximants for $(v_c - v)\mathrm{d}[\ln \tilde{\chi}(v)]/\mathrm{d}v$ were evaluated at the chosen v_c, (see Hunter and Baker 1973) and indicate a γ value in the range $1{\cdot}401 \pm 0{\cdot}002$. From this result and table 1, we take $1{\cdot}395$ as a mean estimate for γ.

Table 1. Neville table for the exponent estimate sequence γ_n, defined in equation (2).

		Order of extrapolant				
n	γ_n	1st	2nd	3rd	4th	5th
4	1·0472					
5	1·1119	1·3706				
6	1·1569	1·3821	1·4049			
7	1·1901	1·3900	1·4060	1·4074		
8	1·2152	1·3910	1·3974	1·3829	1·3585	
9	1·2348	1·3919	1·3951	1·3906	1·4002	1·4336
10	1·2506	1·3923	1·3937	1·3903	1·3899	1·3796

To calculate the γ uncertainty, the above procedure was repeated using instead a v_c value at one end of its uncertainty range. With $v_c = 0{\cdot}2373$ we obtained $\gamma = 1{\cdot}420 \pm 0{\cdot}005$ from the Neville table and $\gamma = 1{\cdot}428 \pm 0{\cdot}003$ from the Padé approximants. We thus take $\gamma = 1{\cdot}395 \pm 0{\cdot}030$ as our final estimate.

The susceptibility series for the spin-$\frac{1}{2}$ model on the BCC and FCC lattices, and for the classical model on the SC and BCC lattices were treated in the same way, and the results for K_c and γ are summarized in table 2. There appears to be general consistency among the various γ estimates; in particular, the table shows no significant difference, outside the uncertainties, between the values for the spin-$\frac{1}{2}$ and classical models. Thus our results support the universality hypothesis, and we take $\gamma = 1{\cdot}40 \pm 0{\cdot}02$ for both models. In view of the shortness of the series we do not believe the value can be quoted more precisely than this.

The implications of $\gamma = 1{\cdot}4$ for the other exponent values have already been discussed by Ferer *et al* (1971) and by Rushbrooke *et al* (1974). Without reiterating

Table 2. Estimates for the inverse critical temperature K_c and susceptibility exponent γ for the spin-$\frac{1}{2}$ and classical (spin infinity) models on the three cubic lattices. †The classical FCC values are those of Ferer *et al* (1971), a transformation analysis being inappropriate for this case.

Series	K_c	γ
Spin-$\frac{1}{2}$		
SC	$0{\cdot}5942 \pm 0{\cdot}0020$	$1{\cdot}395 \pm 0{\cdot}03$
BCC	$0{\cdot}3965 \pm 0{\cdot}0020$	$1{\cdot}41 \pm 0{\cdot}04$
FCC	$0{\cdot}2485 \pm 0{\cdot}0007$	$1{\cdot}405 \pm 0{\cdot}035$
Classical		
SC	$0{\cdot}6940 \pm 0{\cdot}0020$	$1{\cdot}415 \pm 0{\cdot}03$
BCC	$0{\cdot}4870 \pm 0{\cdot}0005$	$1{\cdot}40 \pm 0{\cdot}03$
FCC†	$0{\cdot}3149 \pm 0{\cdot}0002$	$1{\cdot}405 \pm 0{\cdot}020$

them in detail, we note that it is possible to sharpen them somewhat by making a new estimate of $2\nu-\gamma$ from the series for $\mu_2(K)/(\chi(K))^2$ where $\mu_2(K)$ is the second moment of the correlation function (see Ritchie and Fisher 1972). This function is expected to be singular at the critical point with exponent $2\nu-\gamma$, and Padé estimates for this (obtained in the same way as for γ above) are given in table 3 for the classical Heisenberg model on the FCC lattice. (The corresponding table for the BCC lattice gave similar estimates, but that for the SC lattice showed too much scatter to be useful.) If we take $2\nu-\gamma$ to be $0\cdot025\pm0\cdot001$ on the basis of these tables, we obtain a value of $0\cdot712\pm0\cdot012$ for ν; application of the Fisher equation (Fisher 1964), $\gamma=(2-\eta)\nu$, then leads to $\eta=0\cdot035\pm0\cdot003$.

Table 3. Padé approximants to $(K_c-K)\mathrm{d}[\ln(\mu_2(K)/(\chi(K))^2)]/\mathrm{d}K$ evaluated at K_c, for the classical Heisenberg model on the FCC lattice. The values of these approximants should give estimates for $2\nu-\gamma$. '*a*' indicates an approximant with a defect on the positive real axis, '*b*' one with a negative real axis defect, and '*c*' one with a pair of defects off the real axis.

L \ M	2	3	4	5	6
2	0·02504	0·02499	0·02442	0·02481	0·02517*b*
3	0·02500	0·02504*a*	0·02463	0·02376*a*	
4	0·02294	0·02469	0·02480*c*		
5	0·02458	0·02466*c*			
6	0·02349*a*				

These estimates for the correlation exponents are consistent with those of Ritchie and Fisher, and Ferer *et al*, but that for η carries a significantly smaller uncertainty. (These author's estimates were $\eta=0\cdot043\pm0\cdot014$ and $0\cdot040\pm0\cdot008$ respectively.) The conclusion that the exponent values are consistent with scaling remains unchanged of course from that of Ferer *et al*, but we observe that the comparatively precise result for η implies that either δ must be slightly less than the appealing value of 5·0, or the dimension dependent relation of Gunton and Buckingham (1968) and Fisher (1969): $2-\eta\leqslant d(\delta-1)/(\delta+1)$ must hold as a strict inequality.

More details of the γ and K_c estimation for the other lattices, together with formal justification of the transformation methods employed, will be given in a later publication.

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