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Confluent corrections to scaling in the isotropic Heisenberg model†

William J Camp and J P Van Dyke
Sandia Laboratories, Albuquerque, New Mexico 87115, USA

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Abstract. Confluent corrections to scaling are explicitly incorporated in the analysis of high-temperature series for the $S=\frac{1}{2}$ (quantum-mechanical) and $S=\infty$ (classical) isotropic Heisenberg models on the FCC lattice. For $S=\infty$, strong confluent corrections are found in the susceptibility, the second moment of the correlation function, as well as the anisotropy crossover function. No evidence for confluent, non-analytic corrections to scaling is found in our analysis of the $S=\frac{1}{2}$ susceptibility. Our best value for the $S=\infty$ susceptibility exponent is $\gamma(\infty)=1{\cdot}42^{+0{\cdot}02}_{-0{\cdot}01}$, which—taken with the best previous estimate $\gamma(\frac{1}{2})=1{\cdot}43$—is consistent with universality. However, for $S=\frac{1}{2}$, we feel that (because of apparent non-confluent singularities) γ is known no better than $\gamma(\frac{1}{2})\approx 1{\cdot}41$–$1{\cdot}51$. The $S=\infty$ correlation-length exponent is estimated to be $\nu=0{\cdot}725\pm0{\cdot}015$, and the crossover exponent is estimated to be $\phi=1{\cdot}30\pm0{\cdot}03$. Finally, the $S=\infty$ correction-to-scaling exponent is found to be $\Delta_1=0{\cdot}54\pm0{\cdot}10$.

1. Introduction

The status of our understanding of critical behaviour in the spin-S isotropic Heisenberg model has recently been extensively reviewed by Rushbrooke, Baker and Wood (Rushbrooke *et al* 1974). A problem left unresolved by them was the apparent lack of a universal value for the susceptibility exponent γ of the Heisenberg model: Padé analysis of the $S=\frac{1}{2}$ series has yielded the estimate $\gamma(\frac{1}{2})=1{\cdot}43\pm0{\cdot}01$ (Baker *et al* 1967), whereas, in contrast, estimates for $S=\infty$ are no greater than $\gamma(\infty)=1{\cdot}405\pm0{\cdot}02$ (Ferer *et al* 1971), as low as $\gamma(\infty)=1{\cdot}36\pm0{\cdot}04$ (Lee and Stanley 1971), and more recently $\gamma(\infty)=1{\cdot}375^{+0{\cdot}02}_{-0{\cdot}01}$ (Ritchie and Fisher 1972). Ritchie and Fisher (1972) proposed that their estimate was valid for all S. However, in so doing they chose to ignore evidence for a larger exponent at $S=\frac{1}{2}$, citing the poorer apparent convergence of the $S=\frac{1}{2}$ series. Lee and Stanley concluded that their estimate $\gamma=1{\cdot}36$ also applied for $S=\frac{1}{2}$. However, Rushbrooke *et al* (1974) have pointed out that closely related methods of analysis do not support this conclusion.

We have re-examined both the $S=\frac{1}{2}$ and $S=\infty$ series using methods previously employed to study the spin-S Ising susceptibility (Camp and Van Dyke 1975a, Saul *et al* 1975) and pair correlation function (Camp *et al* 1975) which explicitly allows for the existence of non-analytic confluent corrections to the dominant critical behaviour, as for example in the susceptibility,

$$\chi\approx\chi_0/(1-T_c/T)^{\gamma}+\chi_1/(1-T_c/T)^{\gamma-\Delta_1}. \qquad (1)$$

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Although such corrections are predicted by renormalization group theory to be important corrections to the dominant scaling behaviour (Wegner 1972), no previous attempts to identify and remove these corrections have been made in the case of the Heisenberg model. In view of the comparative shortness of all series analysed, the results reported below cannot be regarded as completely conclusive.

We conclude from our analysis that much of the difference between the exponents previously estimated for $S=\infty$ and $S=\frac{1}{2}$ is due to the presence of rather strong confluent corrections to scaling in the $S=\infty$ susceptibility. Nevertheless, incorporation of such corrections does not completely satisfactorily lead to a single, best universal value for γ. This is apparently due to the importance of non-confluent corrections which have eluded successful analysis (see, however, Rushbrooke *et al* 1974, p 327). On this point it is worth noting that although for $S=\frac{1}{2}$ the estimate $\gamma(\frac{1}{2})=1{\cdot}43$ by Baker *et al* (1967) represents a reasonable 'best' value, it does indicate a bias toward lower values for γ. Indeed, extrapolations based on both simple and extended ratio methods (as well as estimates based on the corners of the very Padé tables upon whose centres Baker *et al* (1967) based their estimates) lead to somewhat higher estimates for $\gamma(\frac{1}{2})$ in the range $\gamma(\frac{1}{2})\approx 1{\cdot}45$–$1{\cdot}50$. This poor convergence is not due to confluent corrections (we find none for $S=\frac{1}{2}$), rather it must be due to non-confluent singularities. For $S=\infty$, the results of previous analyses appear less confusing in that estimates based on simple and extended ratio methods as well as Padé estimates are found to be mutually consistent, fairly well converged, and in the somewhat narrower range $\gamma(\infty)\approx 1{\cdot}38$–$1{\cdot}41$.

We summarize our susceptibility analysis as follows. (i) We find no evidence for confluent corrections at $S=\frac{1}{2}$ based on extrapolation of available ninth-order series. (ii) Using the confluent singularity analysis described below, and accepting the estimate of Baker *et al* (1967) for the critical point, we find $\gamma(\frac{1}{2})\approx 1{\cdot}43^{+0{\cdot}01}_{-0{\cdot}02}$ but with considerable scatter. (iii) Using the confluent singularity analysis, but adjusting the critical point to minimize the scatter in estimates (see below), we find $\gamma(\frac{1}{2})\approx 1{\cdot}50\pm 0{\cdot}02$ (with comparatively little scatter). (iv) For $S=\infty$ we use available tenth-order series, and all methods employed point to a rather strong confluent correction term. The correction exponent associated with this term is given by $\Delta_1=0{\cdot}54\pm 0{\cdot}10$ (see below). (v) Most of the $S=\infty$ analysis performed points to a critical point within $0{\cdot}1\%$ of the previous estimates by Ferer *et al* (1971) and by Ritchie and Fisher (1972). For critical points in this range we obtain estimates, with relatively little order-by-order scatter, in the range $\gamma(\infty)\approx 1{\cdot}42^{+0{\cdot}02}_{-0{\cdot}01}$. (vi) There is slight evidence for a significantly different $S=\infty$ critical point with correspondingly higher exponent $\gamma(\infty)\approx 1{\cdot}48$. In this case the correction exponent is unchanged, but the strength of the correction term is greatly enhanced. However, in the light of analysis of the second moment of the pair correlation function described below which strongly favours the accepted critical point, we believe that the evidence for $\gamma(\infty)\approx 1{\cdot}48$ is weak indeed.

With regard to points (ii) and (iii) above, since we find no evidence of a confluent singularity we would *not* propose that for $S=\frac{1}{2}$ the results of our extended analysis are any more valid than those based on simple ratio and Padé analysis. Indeed they simply reflect the already existing dichotomy in the results of straightforward ratio and Padé analyses which we discussed above.

For $S=\infty$ we have also re-analysed existing tenth-order series for the second moment of the pair correlation function (Ferer *et al* 1971) and tenth-order series for the anisotropy crossover function (Camp and Van Dyke 1974). The analysis of these series again confirms the existence of confluent corrections to scaling. For both the second moment and the crossover function, no evidence is found for a critical temperature significantly different from that previously estimated for $S=\infty$ (Ferer *et al* 1971, Ritchie and Fisher 1972). The estimates for the correction exponent are quite scattered (especially in the case of the crossover function), but certainly consistent with the estimate $\Delta_1 \approx 0{\cdot}54 \pm 0{\cdot}10$ obtained from the susceptibility. From the second moment analysis we find the correlation length exponent to be $\nu = 0{\cdot}725 \pm 0{\cdot}015$ (compare with previous estimates: $\nu = 0{\cdot}705 \pm 0{\cdot}008$ (Ritchie and Fisher 1972) and $\nu = 0{\cdot}717 \pm 0{\cdot}007$ (Ferer *et al* 1971)). Using the scaling relation $\eta = 2 - \gamma/\nu$ we estimate the anomalous correlation exponent to be $\eta \approx 0{\cdot}04$, with large uncertainty. The anisotropy crossover exponent ϕ is estimated from the crossover function $\chi(g)^{-1}\partial\chi(g)/\partial g(g \to 0)$,where g is the spin anisotropy parameter (see below). The crossover exponent is found to be $\phi = 1{\cdot}30 \pm 0{\cdot}03$, which because of corrections to scaling differs considerably from the previous estimate $\phi = 1{\cdot}25$ based on straightforward ratio and Padé analyses (Pfeuty *et al* 1974).

2. Methods and assumptions

The basic assumption of the analysis presented herein is that corrections to the dominant scaling behaviour are either confluent with the dominant scaling behaviour, or analytic, or both. As we have discussed, there is ample evidence, for spin-half especially, that this assumption is not completely valid. However, since (on the close-packed FCC net) confluent corrections should generally dominate non-confluent ones, and since the short length of available series prohibits any reasonable accounting for non-confluent corrections, we accept the assumption unchanged.

Confluent, non-analytic corrections to scaling were first predicted on empirical grounds by M Wortis (1970, paper presented at *Newport Beach Conf. on Phase Transitions, January* 1970, unpublished). The justification of Wortis' arguments by detailed renormalization group calculations has been presented by Wegner (1972), who showed that the dominant scaling behaviour is generalized to a scaling function of several variables. For example, in the case of the pair correlation function it is expected that

$$G(\boldsymbol{R}) \approx R^{-(d-2+\eta)}\tilde{G}(R\tau^{\nu}, RH^{\nu/\Delta}, Rg^{\nu/\phi}, Ru^{-\nu/\Delta_1}, \ldots) \tag{2}$$

where d is the lattice dimension, H the magnetic field, $\Delta(=\frac{1}{2}(2+\gamma-\alpha))$ the gap exponent, u the leading 'irrelevant' field, and $\tau(=1-T_c/T)$ the reduced distance from the critical point. The variables η, ν, ϕ, and g are as above. The susceptibility is obtained as the zeroth spatial moment of $G(R)$ using the fluctuation theorem. The moments μ_m are defined as

$$\mu_m \equiv \int \mathrm{d}^d R |R|^m G(R) \approx \int_0^{\infty} \mathrm{d}R\, R^{m+1-\eta}\tilde{G}(R\tau^{\nu}, RH^{\nu/\Delta}, Rg^{\nu/\phi}, Ru^{-\nu/\Delta_1}, \ldots). \tag{3}$$

By changing the integration variable to $R\tau^{\nu}$ in the integral, we obtain

$$\mu_m = \tau^{-\nu(m+2-\eta)}\tilde{M}_m(H/\tau^{\Delta}, g/\tau^{\phi}, u\tau^{\Delta_1}, \ldots). \tag{4}$$

The scaling function $\tilde{G}$ is assumed to be an analytic function of its arguments; hence also is $\tilde{M}_m$. The three functions of interest herein—the susceptibility, second moment and crossover function—may all be derived from equation (4). Consider first the isotropic

($g=0$), zero-field ($H=0$) susceptibility. We employ a Taylor expansion to obtain

$$\chi \equiv \mu_0 \approx \tau^{-(2-\eta)\nu}(\chi_0 + \chi_{1u} u\tau^{\Delta_1} + \ldots). \tag{5}$$

We identify γ as $\gamma=(2-\eta)\nu$ and see that a secondary divergence $\tau^{-\gamma+\Delta_1}$ is predicted. Likewise the second moment is given, for $g=H=0$, by

$$\mu_2 \approx \tau^{-(\gamma+2\nu)}(M_{2,0} + M_{2,u} u\tau^{\Delta_1} + \ldots). \tag{6}$$

The crossover function is given by

$$\chi^{-1}\frac{\partial \chi}{\partial g}\bigg|_{g=0} \approx \tau^{-\phi} \lim_{x\to 0}\left((\tilde{M}_0(0, x, u\tau^{\Delta_1}, \ldots))^{-1}\frac{\partial}{\partial x}\tilde{M}_0(0, x, u\tau^{\Delta_1}, \ldots)\right)$$
$$= \tau^{-\phi}(\chi_{1g}/\chi_0)(1 + Au\tau^{\Delta_1} + \ldots) \tag{7}$$

where we have used the Taylor series representation for $\tilde{M}_0(x_1, x_2, \ldots)$. To summarize, for a given model renormalization group theory predicts confluent corrections to dominant scaling with the same exponent for all functions, but with correction amplitudes varying from function to function.

Two methods of series analysis have been developed and successfully applied to analyse and remove confluent corrections. In the method of four-fits (Moore *et al* 1974, Saul *et al* 1975, Camp and Van Dyke 1975a) the value of T_c (or γ) is specified and successive estimates for γ (or T_c), Δ_1, χ_0, and χ_1 are obtained by direct fitting of equation (1) to series coefficients. In the Baker–Hunter transformation (Baker and Hunter 1973, Camp and Van Dyke 1975a) T_c is employed as an input parameter to a non-linear series transformation which provides accurate estimates for γ, Δ_1, χ_0, and χ_1.

The four-fit procedure involves the solution of four simultaneous non-linear equations for the fitting parameters in terms of four consecutive coefficients, f_{n-3}, f_{n-2}, f_{n-1}, and f_n, of the high-temperature series involved. Thus sets of estimates are obtained for $n=3, 4, 5, \ldots$ up to the highest order for which the series coefficient is available.

The Baker–Hunter transformation is described in some detail by Camp and Van Dyke (1975a). Here, we outline it only briefly. Consider equation (5) above with $\tau = 1-K/K_c(K=J/kT)$. Introduce a variable $\xi = -\ln(1-K/K_c)$. Using the first N terms in the high-temperature series for $\chi(K)$, form the first N terms in the series for $\chi(\xi) \approx \chi_0\,e^{\gamma\xi} + \chi_1\,e^{(\gamma-\Delta_1)\xi}$. Multiply the nth term in the series for $n=0, 1, 2, \ldots N$ by $n!$ to form the series for the auxiliary function $\mathscr{F}(\xi) \approx \chi_0/(1-\gamma\xi) + \chi_1/[1-(\gamma-\Delta_1)\xi]$. The poles of the direct Padé approximants to $\mathscr{F}(\xi)$ determine γ and Δ_1, as well as the exponents of any weaker confluent singularities; and their residues determine the amplitudes χ_0, χ_1, etc. In particular, if χ is exactly of the form in equation (5), to within analytic corrections, the sequence of $[N-1/N]$ Padé approximants should provide especially rapidly convergent estimates (Baker and Hunter 1973, Camp and Van Dyke 1975a). (See, however, below.)

In the case of the spin-S Ising model both methods have yielded accurate estimates for the critical parameters which provide striking evidence for the universality (with spin) of γ and Δ_1 in the Ising model (Camp and Van Dyke 1974, Saul *et al* 1975). In addition studies of the second moment of the FCC spin-S Ising pair correlation function (Camp *et al* 1975) confirm the structure of the corrections to scaling as well as the universality with spin of the correlation-length exponent, ν. The Heisenberg series analysed herein are uniformly more poorly converged than their counterpart Ising series. Nonetheless we believe the results herein provide clear evidence for the existence of confluent corrections at $S=\infty$, and for their absence at $S=\frac{1}{2}$.

In both our four-fit and Baker–Hunter analysis we treat the critical point $K_c(=J/kT_c)$ as an input parameter. We may choose K_c to maximize the apparent convergence of the sequence of estimates for the critical-point parameters; or we may restrict K_c to a relatively narrow range about the best previous estimates from ratio and Padé analyses and examine the convergence and spread of estimates in that range. Further we can choose for empirical reasons to emphasize one aspect of the analysis. When all these options are taken into account, the range of allowed values, say for γ, is rather large. However, if we are willing to restrict severely the range of allowed values for K_c, the apparent spread in exponents is quite narrow—comparable to the ranges found in previous biased analyses (see Rushbrooke *et al* 1974).

3. The Hamiltonian and series

The anisotropic quantum-mechanical Heisenberg Hamiltonian is given by

$$-\beta\mathcal{H}=(K/S^2)\sum_{\langle ij\rangle}\sum_{\mu=1}^{3}\eta_\mu S_i^\mu S_j^\mu.$$

For $\eta_1=\eta_2=\eta_3=1$, we recover the isotropic Heisenberg model. For $S=\frac{1}{2}$ (the full quantum limit), ninth-order series in K are available for the isotropic susceptibility on the FCC net (Baker *et al* 1967). For $S=\infty$, tenth-order series for the anisotropic susceptibility have been derived as analytic functions of η_1, η_2, and η_3 by Camp and Van Dyke (1974) on all standard lattices. In addition these authors have derived series for the pair correlation function and moments (again as analytic functions of η_1, η_2, and η_3) through ninth order on the FCC net, and through tenth order on the remaining standard two- and three-dimensional lattices (Camp and Van Dyke 1975b). Using the identifications $\eta_1=1+g$, $\eta_2=1-g$, $\eta_3=1$ (rhombic anisotropy) or $\eta_1=1+g$, $\eta_2=\eta_3=1-\frac{1}{2}g$ (axial anisotropy) we may easily construct crossover functions (see further Pfeuty *et al* 1974). For $S=\frac{1}{2}$, the anisotropic series, as well as the isotropic series for the moments and correlation function, are of insufficient length to be analysed by the methods used herein.

Since the various series analysed are in the literature, we do not repeat them. One exception is the crossover function, for which Pfeuty *et al* (1974) only derived the FCC series through eighth order. For completeness we give, in the relevant section below, the series coefficients through tenth order which are used in our analysis.

4. Analysis of the spin-half susceptibility

The Padé analysis of this series is thoroughly discussed by Baker *et al* (1967). The conclusion by these authors that $K_c(\frac{1}{2})=0{\cdot}2492$ and $\gamma(\frac{1}{2})=1{\cdot}43\pm0{\cdot}01$ rests on three sets of results. First (Baker *et al* 1967, method (i)) the [6/2], [5/3], [4/4], and [3/5] Padé approximants, the centre of the outermost diagonal of the Padé table, to $\mathrm{d}\ln(\chi)/\mathrm{d}K$ yield the estimates $K_c(\frac{1}{2})=0{\cdot}2492\pm0{\cdot}0001$, and $\gamma(\frac{1}{2})=1{\cdot}428\pm0{\cdot}006$. However, it should be noted that the [8/0], [7/1], [2/6], and [1/7] approximants to this function, which employ the same number of coefficients from the series as those mentioned above, provide estimates $K_c(\frac{1}{2})=0{\cdot}2503\pm0{\cdot}0002$ and $\gamma(\frac{1}{2})=1{\cdot}484\pm0{\cdot}012$.

Further if we average over all $[n/m]$ Padé approximants with $N=n+m$ (neglecting obvious defects) we obtain the succession of estimates $\langle\gamma(\frac{1}{2})\rangle_N = 1{\cdot}214$, $1{\cdot}313$, $1{\cdot}355$, $1{\cdot}460$, and $1{\cdot}456$ for $N=4$, 5, 6, 7, and 8, respectively. The apparent spread $\langle\gamma(\frac{1}{2})\rangle_8 = 1{\cdot}46^{+0{\cdot}03}_{-0{\cdot}04}$ is typical of the higher-order averages. Likewise, we can average $K_c(\frac{1}{2})$ to find $\langle K_c(\frac{1}{2})\rangle_N = 0{\cdot}2417$, $0{\cdot}2454$, $0{\cdot}2465$, $0{\cdot}2501$, $0{\cdot}2497$ for $N=4$, 5, 6, 7, and 8, respectively. One can reasonably argue that the centre of the Padé table is sometimes found to be more rapidly converged than the corners, so that one should not weigh the corner estimates strongly. Nonetheless the higher exponents found in averaging over a diagonal have a smooth order-to-order variation and certainly indicate a minimal reasonable spread about the central estimate, $\gamma = 1{\cdot}43$, quoted by Baker *et al* (1967).

The second piece of evidence used by Baker *et al* (1967) was the remarkable consistency between the estimates $\gamma(\frac{1}{2}) = 1{\cdot}43$ and $K_c(\frac{1}{2}) = 0{\cdot}2492$ (Baker *et al* 1967, methods (ii) and (iii)). The Padé approximants to $(K-0{\cdot}2492)\mathrm{d}\ln\chi/\mathrm{d}K$ approach $1{\cdot}430$ at $K=0{\cdot}2492$ with high precision for nearly all higher-order approximants. Similarly the dominant poles in the Padé approximants to $(\chi)^{1/1{\cdot}43}$ reproduce $K_c(\frac{1}{2}) = 0{\cdot}2492$ with high accuracy in nearly all higher-order approximants. However, as noted by Baker *et al* (1967), this apparent high convergence is deceptive since a higher (lower) choice of $K_c(\frac{1}{2})$ produces consistent, well converged higher (lower) estimates for $\gamma(\frac{1}{2})$. Therefore the evidence from these methods is not as strong as that from the first method above.

Perhaps the strongest evidence for $\gamma(\frac{1}{2}) = 1{\cdot}43$ presented by Baker *et al* (1967) lay in their analysis of

$$\frac{\mathrm{d}}{\mathrm{d}K}\left(\ln\frac{\mathrm{d}\chi}{\mathrm{d}K}\right)\left(\frac{\mathrm{d}}{\mathrm{d}K}\ln\chi\right)^{-1} \to \frac{\gamma+1}{\gamma}$$

as $K \to K_c(\frac{1}{2})$ (Baker *et al* 1967, method (iv)). Using the [4/2], [5/2], [4/3], and [3/4] approximants they find that $\gamma = 1{\cdot}427 \pm 0{\cdot}008$ *nearly independent of the choice of* $K_c(\frac{1}{2})$ over the range $0{\cdot}246 \leqslant K_c(\frac{1}{2}) \leqslant 0{\cdot}249$. This is quite good evidence for $\gamma = 1{\cdot}43$. Nevertheless, as with the analysis of $\mathrm{d}\ln\chi/\mathrm{d}K$, the [6/0], [7/0], [6/1], and [1/6] approximants paint a somewhat different picture. Namely, $\gamma = 1{\cdot}495 \pm 0{\cdot}015$, also *independent of the choice of* K_c *in the above range.* As with the logarithmic-derivative analysis above, the average is $\langle\gamma(\frac{1}{2})\rangle \approx 1{\cdot}46 \pm 0{\cdot}04$. Here the average and the spread are explicitly independent of $K_c(\frac{1}{2})$ in the range $0{\cdot}246 \leqslant K_c \leqslant 0{\cdot}249$. Seen in this light, the evidence from method (iv) of Baker *et al* is nearly identical to that from their method (i): considerable evidence for $\gamma \approx 1{\cdot}43$ or $\gamma = 1{\cdot}49$ with a 'compromise' choice $\gamma \approx 1{\cdot}46$. We have re-examined their series analysis of

$$\frac{\mathrm{d}}{\mathrm{d}K}\left(\ln\frac{\mathrm{d}\chi}{\mathrm{d}K}\right)\left(\frac{\mathrm{d}}{\mathrm{d}K}(\ln\chi)\right)^{-1}$$

and conclude that nothing in the above discussion is changed by extension of their range for $K_c(\frac{1}{2})$ to $0{\cdot}2460 \leqslant K_c(\frac{1}{2}) \leqslant 0{\cdot}2520$, i.e., double the range discussed by Baker *et al* (1967).

Finally, with regard to these results, it is useful to compare with similar analyses of the well behaved spin-half Ising susceptibility series on the FCC net. The analyses of

$$\frac{\mathrm{d}}{\mathrm{d}K}(\ln\chi) \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}K}\left(\ln\frac{\mathrm{d}\chi}{\mathrm{d}K}\right)\left(\frac{\mathrm{d}}{\mathrm{d}K}(\ln\chi)\right)^{-1}$$

by Padé approximants are particularly clean for this model. For example, the Padé analysis of the latter function, using any $[l/m]$ approximant with $l+m=6, 7, 8, 9$, and 10, yields estimates for γ_I of $1{\cdot}249 \pm 0{\cdot}001$, $1{\cdot}246 \pm 0{\cdot}002$, $1{\cdot}2477 \pm 0{\cdot}0005$, $1{\cdot}2476 \pm 0{\cdot}0003$, and $1{\cdot}2476 \pm 0{\cdot}0003$, respectively. The quoted uncertainty represents the sum of the uncertainty due to the variation of γ_I from approximant to approximant at fixed K_c^I and fixed $l+m$, and the uncertainty due to the variation of γ_I with the assumed value of K_c^I in the range $0{\cdot}09411 \leq K_c^I \leq 0{\cdot}09597$ centred about the 'best' estimate $K_c^I = 0{\cdot}09504$ (Camp and Van Dyke 1975a). In particular no evidence is found in the analysis of this series to favour either the centre or the corners of the Padé table. Convergence of the $[l/m]$ approximants apparently does not depend on l and m separately, but only on the sum $l+m$. The implication of this result is that it is premature to discard the estimate $\gamma(\frac{1}{2}) \approx 1{\cdot}48$ from the corners of the Padé tables in favour of the estimate $\gamma(\frac{1}{2}) \approx 1{\cdot}43$ from centres of the tables.

Baker *et al* (1967) do not explicitly discuss ratio analysis of the $S=\frac{1}{2}$ susceptibility, except to state that ratio analysis generally confirms the Padé analysis. We have examined the ratios of successive series coefficients using linear extrapolants, higher-order Neville tables and the method of end-shifts. Analyses were performed: (i) with neither γ nor K_c specified; (ii) specifying K_c and estimating γ; and (iii) specifying γ and estimating K_c. When neither K_c nor γ are specified both higher-order Neville tables and end-shift estimates are too scattered to be useful. However, straightforward linear extrapolants provide estimates $\{\gamma(\frac{1}{2}); K_c(\frac{1}{2})\} = \{1{\cdot}363; 0{\cdot}2466\}$, $\{1{\cdot}397; 0{\cdot}2479\}$, $\{1{\cdot}440; 0{\cdot}2494\}$, and $\{1{\cdot}454; 0{\cdot}2498\}$ in sixth, seventh, eighth, and ninth orders, respectively. These estimates, albeit poorly converged, are apparently increasing beyond $\{\gamma(\frac{1}{2}); K_c(\frac{1}{2})\} = \{1{\cdot}43; 0{\cdot}2492\}$. The biased analyses, methods (ii) and (iii), are typified by the linear extrapolant estimates for $\gamma(\frac{1}{2})$, given $K_c(\frac{1}{2})$. The best behaved sequence is perhaps that for $K_c(\frac{1}{2}) = 0{\cdot}2497$ for which we find the estimates $\gamma(\frac{1}{2}) = 1{\cdot}50$, $1{\cdot}45$, $1{\cdot}42$, $1{\cdot}43$, $1{\cdot}44$, $1{\cdot}45$, $1{\cdot}45$, and $1{\cdot}45$ using orders 2 through 9, respectively. However, convergence of the sequence does not fall off very much in the range $0{\cdot}2491 \leq K_c(\frac{1}{2}) \leq 0{\cdot}2505$ for which $\gamma(\frac{1}{2})$ varies from $1{\cdot}43$ at the lower end of the range to $1{\cdot}48$ at the upper end. Thus, as with various Padé methods, we fail to obtain any single best estimate for $K_c(\frac{1}{2})$ or $\gamma(\frac{1}{2})$ from ratio analysis.

4.1. *Confluent-singularity analysis*

The method of four-fits breaks down for the $S=\frac{1}{2}$ susceptibility. A problem is that the correction exponent Δ_1 is poorly determined (i.e., exhibits great order-to-order variation and fails to remain within any physically reasonable range). This is apparently due to the fact that confluent corrections are either very small (and thus poorly determined in analysis based on short series) or completely absent. This interpretation of the breakdown of four-fits is consistent with the Baker–Hunter analysis which produces no secondary singularity (or, at least no *non-analytic* correction—see below), but which in contrast to four-fits does not break down completely.

As pointed out by Baker and Hunter (1973) for functions with *only* confluent singularities the sequence of $[N-1/N]$ Padé approximants to $\mathscr{F}(\xi)$ provides particularly rapidly convergent estimates for the amplitudes and exponents of the singularities. In our analysis of the spin-S Ising susceptibility (Camp and Van Dyke 1975a) we thus relied mainly on analysis using $[N-1/N]$ approximants to the transformed series $\mathscr{F}(\xi)$—although, for that model, the table as a whole agrees well with the $[N-1/N]$ sequence. For test series with analytic noise and/or non-confluent corrections in addition to confluent singularities, we have since found that it is often best to rely on trends involving the Padé table as a whole, rather than just the $[N-1/N]$ sequence. For the spin-half Heisenberg susceptibility there is no real difference between the $[N-1/N]$ sequence and the remainder of the table. However for the spin-infinity susceptibility the 'best' choice of K_c based on convergence of the Padé table as a whole fails to agree with that based on the convergence of the $[N-1/N]$ sequence of approximants. Furthermore, the two convergence criteria lead to markedly different estimates for $\gamma(\infty)$. We shall pursue this further below in the discussion of the $S=\infty$ susceptibility.

In table 1 we list the Baker–Hunter estimates for γ and χ_0 obtained by assuming $K_c = 0{\cdot}2519$. This set of results exhibits the best apparent convergence obtained for any choice of $K_c(\frac{1}{2})$, based both on the $[N-1/N]$ sequence, and on the Padé table as a whole. The apparent value of $\gamma(\frac{1}{2})$ is $1{\cdot}50 \pm 0{\cdot}02$, and the estimated dominant amplitude is $\chi_0 = 1{\cdot}01 \pm 0{\cdot}02$. The quality of apparent convergence is retained in the range $K_c(\frac{1}{2}) = 0{\cdot}2519 \pm 0{\cdot}0003$, and falls off quite gradually outside that range. For $K_c(\frac{1}{2})$ in the above range the central estimates for γ lie in the range $\gamma(\frac{1}{2}) = 1{\cdot}50 \pm 0{\cdot}01$. Although no confluent singularities are detected, all approximants with three or more poles are marred by pairs of complex poles located closer to the origin than γ^{-1}. These poles are nearly cancelled by associated sets of zeros, so that the residues of the defects are $O(10^{-3})$ or less. As discussed by Camp and Van Dyke (1975a) such complex defects in the transformed series can be indicative of interfering non-confluent singularities.

Table 1. Baker–Hunter analysis of $\chi(\frac{1}{2})$ with $K_c(\frac{1}{2}) = 0{\cdot}2519$. Most approximants have defects in the complex plane (see text). In each entry γ is listed above χ_0. No real poles representing weaker singularities were found.

M \ N	2	3	4	5	6	7
2	1·442 1·108	1·498 1·005	1·504 0·997	1·499 1·008	1·552	1·613
3	1·448 1·095	1·504 0·996	1·502 1·003	1·504 0·997	1·484 1·033	
4	1·742 0·508	1·499 1·008	1·504 0·997	1·500 1·004		
5	1·705 0·568	1·559 0·862	1·487 1·034			
6	—	1·656 0·644				
7	—					

A very significant aspect of table 1 is the value of $K_c(\frac{1}{2})$. This value, 0·2519, is more than 1% away from the best choice $K_c(\frac{1}{2}) = 0{\cdot}2492$ of Baker *et al* (1967). The Baker-

Hunter analysis of $\chi(\frac{1}{2})$ with $K_c(\frac{1}{2})$ set equal to 0·2492 is presented in table 2. These results are similar to those in table 1 in that every entry with three or more poles is marked by a complex defect structure. However the results are more complicated than those of table 1 in the following ways. First the estimates for $\gamma(\frac{1}{2})$ are scattered mainly about two distinct values: $\gamma = 1{\cdot}42 \pm 0{\cdot}01$ and $\gamma = 1{\cdot}46 \pm 0{\cdot}01$. The entries with $\gamma \approx 1{\cdot}46$ have much stronger defects than those with $\gamma \approx 1{\cdot}42$—typically the residues of the defects for $\gamma \approx 1{\cdot}46$ are about two orders of magnitude larger than those for $\gamma \approx 1{\cdot}42$. Further, many (five out of seven) of the entries with $\gamma \approx 1{\cdot}42$ also show a reproducible second pole corresponding to a correction term $\chi_1 \tau^{-(\gamma - \Delta_1)}$ with $\chi_1 \approx 0{\cdot}18$–0·19 and $\Delta_1 \approx 1{\cdot}03$–$1{\cdot}07$. This is consistent with an analytic correction term in the susceptibility. As in table 1 we interpret the complex defects in the Padé table as indicating the existence of rather important non-confluent singularities in $\chi(\frac{1}{2})$.

Table 2. Baker–Hunter analysis of $\chi(\frac{1}{2})$ with $K_c(\frac{1}{2}) = 0{\cdot}2492$. As in table 1, most approximants have defects in the complex plane. Those entries marked with an asterisk have especially strong defects. In each entry γ is listed above χ_0. Those entries marked with a dagger have a secondary pole with $\Delta_1 \approx 1{\cdot}0$ (i.e., an analytic correction).

M \ N	2	3	4	5	6	7
2	1·335 1·084	1·464 1·009*	1·446 1·045*	1·415 1·115†	1·413 1·121†	1·490 0·891
3	1·398 1·142	1·446 1·039*	1·473 1·007*	1·413 1·121†	1·415† 1·115	
4	1·555 0·745	1·419 1·100	1·414 1·114†	1·458 1·013*		
5	1·589 0·671	1·415 1·112	1·419 1·100			
6	—	1·492 0·874				
7	—					

We summarize our 'confluent-singularity' analysis of $\chi(\frac{1}{2})$ as follows. (i) We find no single best value for $\gamma(\frac{1}{2})$: as with standard analyses, evidence is found for $\gamma(\frac{1}{2})$ in the broad range $\gamma \approx 1{\cdot}41$–$1{\cdot}51$. (ii) We find no evidence for any confluent, but non-analytic correction to scaling. (iii) We find rather strong hints that non-confluent terms are the important corrections to scaling in $\chi(\frac{1}{2})$. (iv) It seems reasonable that such non-confluent singularities could account for the failure of methods which do not allow for them to produce convergent estimates for the critical-point parameters. (v) At best, if we require that $K_c(\frac{1}{2})$ lie within a reasonable range (say $\pm 0{\cdot}4\%$) about the best previous estimates, we can conclude that $\gamma(\frac{1}{2})$ is consistent with the choice $\gamma \approx 1{\cdot}43$ due to Baker *et al* (1967). (vi) If we remove the restriction on $K_c(\frac{1}{2})$ we find that a somewhat larger value for $K_c(\frac{1}{2})$—namely $K_c(\frac{1}{2}) \approx 0{\cdot}252$—leads to the best apparent convergence. For $K_c(\frac{1}{2})$ in this range we estimate $\gamma(\frac{1}{2}) \approx 1{\cdot}50 \pm 0{\cdot}02$. (vii) In the light of the absence of confluent singularities the detailed estimates provided by the Baker–Hunter analysis should be given no more weight than previous ratio and Padé analyses.

5. The spin-infinity Heisenberg model

This model is empirically found to be much better behaved than the quantum mechanical, spin-half version of the Heisenberg model. The biased end-shifted ratio estimates for γ vary from $\gamma(\infty)\approx 1{\cdot}389$ at $K_c(\infty)\approx 0{\cdot}31476$ to $\gamma(\infty)\approx 1{\cdot}405$ at $K_c(\infty)\approx 0{\cdot}31496$. The order-to-order scatter in the γ estimates is less than 0·001 for orders eight, nine, and ten throughout the range quoted. The results of Neville-table analysis of ratios (Ferer *et al* 1971) are in very good accord with end-shift analysis.

Despite the apparent smoothness of the sequence of Neville estimates, Ferer *et al* (1971) were able to discern evidence that the series was not completely suited for Neville-table analysis. The point is that Neville-table and end-shift analyses only converge rapidly for sequences of ratios of the form

$$R_n \equiv \chi_n/\chi_{n-1} \approx (K_c)^{-1}[1+(\gamma-1)/n+g_2/n^2+g_3/n^3+\ldots].$$

Neville analysis of sequences in which this analytic dependence on n^{-1} is replaced by, for example, $K_cR_n \approx 1+(\gamma-1)/n+a/n^{3/2}+\ldots$, show distinctive trends from order-to-order, as discussed by Ferer *et al* (1971). These authors noted that the Neville-table analysis of $\chi(\infty)$ showed evidence for just such a non-analytic dependence on n^{-1}. As discussed in detail by Camp and Van Dyke (1975a), non-analytic dependence on n^{-1} (namely $K_cR_n \approx 1+(\gamma-1)/n+a/n^{1+\Delta_1}+\ldots$) is implied by a confluent, but non-analytic, correction term of the form $\chi_1\tau^{-(\gamma+\Delta_1)}$. Thus, already in the discussion of the spin-infinity moments and susceptibility by Ferer *et al* (1971), we find evidence that confluent corrections to scaling enter the $S=\infty$ Heisenberg critical behaviour.

5.1. *Susceptibility analysis—four-fits*

In contrast with $S=\frac{1}{2}$, there is no difficulty in obtaining reasonable four-fit estimates for the $S=\infty$ susceptibility. In table 3 we list the estimates for the parameters χ_0, χ_1, γ and Δ_1 of equation (1) obtained by assuming $K_c(\infty)^{-1}=3{\cdot}174$ ($K_c(\infty)$=0·31506), $K_c(\infty)^{-1}=3{\cdot}175$ ($K_c(\infty)$=0·31496), and $K_c(\infty)^{-1}=3{\cdot}176$ ($K_c(\infty)$=0·31486) (which bracket the 'best' value, $K_c(\infty)^{-1}=3{\cdot}175$, of Ferer *et al* (1971)). We cannot, *a posteriori*, favour any of these three sequences terribly strongly over the others. However, the sequences with $K_c(\infty)$ equal to 0·31496 and 0·31506 are somewhat smoother than that with $K_c(\infty)$ equal to 0·31486. For $K_c(\infty)$=0·31500 the last two sets of four-fit estimates are virtually identical. They are $\gamma=1{\cdot}4296$, $\Delta_1=0{\cdot}543$, $\chi_0=0{\cdot}2296$, and $\chi_1=0{\cdot}1036$. For values of $K_c(\infty)$ outside the range [0·31486, 0·31506] apparent convergence of the four-fit sequences falls off rather noticeably. We thus quote $K_c(\infty)$=0·3150±0·002, $\gamma=1{\cdot}43\pm0{\cdot}03$, $\Delta_1=0{\cdot}54\pm0{\cdot}10$, $\chi_0=0{\cdot}230\pm0{\cdot}050$, and $\chi_1=0{\cdot}104\pm0{\cdot}02$ as our four-fit results. The uncertainties listed are no more than measures of the range over which four-fit sequences are reasonably smooth.

5.2. *Susceptibility analysis—Baker–Hunter transformation*

The best overall convergence of Padé analysis of the Baker–Hunter transformed series is attained when values of $K_c(\infty)^{-1}$ in the range $3{\cdot}175\leqslant K_c(\infty)^{-1}\leqslant 3{\cdot}176$ are employed. Perhaps the 'best' Padé table is that for $K_c(\infty)^{-1}=3{\cdot}1755$ ($K_c(\infty)$=0·31491), which we display in table 4. Even in table 4 the [N/2] and [N/3] approximants are defective for

Table 3. Four-fit analysis of $\chi(\infty)$. Estimate of critical parameters obtained using *N*th order series for $N=5$ through 10 are given.

$K_c(\infty)$	N	γ	Δ_1	χ_0	χ_1
0·31486	5	1·394	0·750	0·267	0·076
	6	1·415	0·558	0·242	0·090
	7	1·433	0·467	0·219	0·108
	8	1·415	0·572	0·242	0·091
	9	1·406	0·674	0·254	0·087
	10	1·403	0·712	0·257	0·088
0·31496	5	1·400	0·720	0·262	0·079
	6	1·427	0·523	0·230	0·100
	7	1·452	0·433	0·199	0·127
	8	1·432	0·507	0·224	0·106
	9	1·422	0·575	0·238	0·097
	10	1·421	0·583	0·239	0·097
0·31506	5	1·406	0·692	0·257	0·083
	6	1·440	0·495	0·218	0·112
	7	1·473	0·411	0·177	0·147
	8	1·452	0·460	0·203	0·125
	9	1·442	0·502	0·216	0·115
	10	1·444	0·492	0·214	0·116

most values of *N*. However the ten 'centre' approximants are very nicely behaved. Using them, we estimate $\gamma=1{\cdot}42^{+0{\cdot}02}_{-0{\cdot}01}$, $\Delta_1=0{\cdot}53^{+0{\cdot}01}_{-0{\cdot}02}$, $\chi_0=0{\cdot}24^{+0{\cdot}01}_{-0{\cdot}02}$, and $\chi_1=0{\cdot}09^{+0{\cdot}01}_{-0{\cdot}02}$. The asymmetrical uncertainties reflect a gradual, but noticeable trend with increasing $N+M$ toward higher values for γ and lower values for Δ_1, χ_0, and χ_1, as estimated from $[N/M]$ approximants. If the choice $K_c(\infty)^{-1}=3{\cdot}1755$ is replaced by 3·175 (3·176) apparent convergence worsens slightly, and the central estimates become $\gamma=1{\cdot}43$ (1·41), $\Delta_1=0{\cdot}49$ (0·62), $\chi_0=0{\cdot}22$ (0·25), and $\chi_1=0{\cdot}10$ (0·08). Thus, apparent convergence is sufficient to quote $\gamma(\infty)=1{\cdot}42\pm0{\cdot}02$ and $\Delta_1=0{\cdot}53^{+0{\cdot}09}_{-0{\cdot}05}$. These estimates agree quite well with the four-fit estimates described above.

Before going on to discuss the second moment of the correlation function, we discuss briefly a quirk in the Baker–Hunter analysis. As mentioned above, for well behaved series (such as that of the spin-infinity Ising susceptibility) the original convergence criterion of Baker and Hunter (1973) based on the sequence of $[N-1/N]$ approximants to $\mathcal{F}(\xi)$ agrees well with that based on convergence of the whole table, and may even converge a little more quickly. However, this is not the case for the $S=\infty$ Heisenberg susceptibility. With $K_c(\infty)^{-1}=3{\cdot}1730$ ($K_c(\infty)=0{\cdot}31516$) the [3/4] and [4/5] approximants yield identical results, namely $\gamma(\infty)=1{\cdot}4425$ and $\Delta_1=0{\cdot}533$. Worse yet, apparent convergence of the entire $[N-1/N]$ sequence is optimized with $K_c(\infty)^{-1}=3{\cdot}1650$ ($K_c(\infty)=0{\cdot}31596$) for which the sequence of estimates for γ from the [1/2] through [4/5] approximants is 1·49, 1·48, 1·49, 1·48, while the sequence of related estimates for Δ_1 is 0·52, 0·54, 0·52, and 0·53. The point here is *not* that $K_c(\infty)=0{\cdot}31596$ is a reasonable choice, but that the series for $\chi(\infty)$ is not terriby 'clean', and probably has non-confluent corrections of some consequence. As pointed out above, for test series when the $[N-1/N]$ sequence convergence criterion disagrees with the overall-table convergence criterion, the latter is generally a more faithful guide to the true behaviour.

Table 4. Padé approximant analysis of the Baker–Hunter transformation of the series for $\chi(\infty)$. The critical point estimate $K_c(\infty)=0{\cdot}31491$ is employed in the transformation. The Padé tables for γ, Δ_1, χ_0, and χ_1 are given sequentially.

γ

M \ N	2	3	4	5	6	7	8
2	1·413	1·126	1·406	1·551	1·366	1·395	1·399
3	1·390	1·406	1·423	1·414	1·417	1·419	
4	1·370	—	1·414	1·416	1·420		
5	1·431	1·377	1·417	1·420			
6	1·413	1·400	1·419				
7	1·386	1·406					
8	1·637						

Δ_1

M \ N	2	3	4	5	6	7	8
2	0·618	—	0·756	—	1·065	—	0·840
3	0·898	0·648	0·555	0·605	0·569	0·545	
4	—	—	0·604	0·583	0·504		
5	0·843	—	0·569	0·500			
6	—	—	0·544				
7	—						
8							

χ_0

M \ N	2	3	4	5	6	7	8
2	0·248	0·383	0·254	0·283	0·293	0·271	0·267
3	0·272	0·254	0·247	0·246	0·241	0·239	
4	0·288	—	0·246	0·242	0·237		
5	0·230	0·285	0·241	0·236			
6	0·251	0·265	0·238				
7	0·284	0·259					
8	0·074						

χ_1

M \ N	2	3	4	5	6	7	8
2	0·088	—	0·083	—	0·019	—	0·019
3	0·102	0·083	0·098	0·089	0·091	0·090	
4	—	—	0·092	0·091	0·080		
5	0·467	—	0·091	0·079			
6	—	—	0·090				
7	—	—					
8	—						

5.3. *Analysis of the second moment of the correlation function*

According to equation (6) we expect the second moment, μ_2, of the pair correlation function to have a dominant singularity with exponent $\gamma+2\nu$ and a secondary singularity which diverges with exponent $\gamma+2\nu-\Delta_1$. We have analysed μ_2, but have preferred to analyse the reduced second moment $\hat{\mu}_2=\mu_2/\chi$ since it removes the problem of choosing γ in order to find ν and Δ_1. Nevertheless, within the accuracy with which we know γ, analysis of μ_2 itself fully confirms that of $\hat{\mu}_2$ discussed herein.

According to equations (5) and (6) we expect that

$$\hat{\mu}_2(\tau)\approx\tau^{-2\nu}(\mu_{2,0}+\mu_{2,1}\tau^{\Delta_1}+\ldots). \qquad (9)$$

This is confirmed by analysis using confluent-singularity techniques. In fact, if anything, apparent convergence of the analysis is better for $\hat{\mu}_2$ than for either χ or μ_2.

First consider the Baker–Hunter transformation. The best apparent convergence of the Padé estimates for 2ν occurs when $K_c(\infty)^{-1}=3{\cdot}1755$ ($K_c(\infty)=0{\cdot}31496$) is used in the transformation. The Padé table with this choice of $K_c(\infty)$ is displayed in table 5. The highest-order diagonals are all consistent with the estimate $2\nu=1{\cdot}440\pm0{\cdot}004$. The apparent convergence of the estimates for the remaining critical parameters is not nearly as good: for Δ_1 we estimate $\Delta_1\approx0{\cdot}6^{+0{\cdot}2}_{-0{\cdot}1}$, while for the amplitudes $\mu_{2,0}$ and $\mu_{2,1}$ we respectively estimate $\mu_{2,0}\approx2{\cdot}8\pm0{\cdot}1$ and $\mu_{2,1}\approx1{\cdot}2\pm0{\cdot}1$. This choice of $K_c(\infty)$ is just that which optimized convergence of the Baker–Hunter estimates for γ. The scatter in the estimates of Δ_1 is disconcerting. However, it should not be of too much concern. For, by choosing $K_c(\infty)^{-1}=3{\cdot}1750$ ($K_c(\infty)=0{\cdot}31496$) as in table 6 we only slightly change the 'best' estimate for 2ν from $1{\cdot}440$ to $1{\cdot}460$, and do not increase seriously the scatter in the estimates. However, a noticeable improvement in the estimates for Δ_1 is obtained. Ignoring the [4/5] approximant (which is defective) we find quite good convergence throughout the centre of the Padé table, and would quote $\Delta_1=0{\cdot}53^{+0{\cdot}07}_{-0{\cdot}10}$.

In summary the Baker–Hunter analysis of $\hat{\mu}_2(\infty)$ agrees with that of $\chi(\infty)$ as regards the 'best' choice of $K_c(\infty)$, and produces estimates for the correction exponent Δ_1 in reasonable accord with those from $\chi(\infty)$. The best value of ν is $\nu\approx0{\cdot}725\pm0{\cdot}015$, while the estimates for Δ_1, $\mu_{2,0}$, and $\mu_{2,1}$ are $\Delta_1\approx0{\cdot}55\pm0{\cdot}10$, $\mu_{2,0}\approx2{\cdot}7\pm0{\cdot}2$, and $\mu_{2,1}\approx1{\cdot}25\pm0{\cdot}15$. Finally we note that in contrast to the Baker–Hunter analysis of $\chi(\infty)$, that of $\hat{\mu}_2(\infty)$ shows no evidence from $[N-1/N]$ Padé analysis for any larger value of $K_c(\infty)$. In particular, the choice $K_c(\infty)=0{\cdot}31596$ leads to scatter of order $0{\cdot}10$ in the $[N-1/N]$ estimates for 2ν.

The four-fit analysis of $\hat{\mu}_2(\infty)$ confirms generally that by Baker–Hunter transformation. In table 7 we show the sequence of estimates found by setting $K_c(\infty)^{-1}$ equal to $3{\cdot}1750$. The sequence is quite smooth, and is consistent with $2\nu=1{\cdot}45\pm0{\cdot}01$, $\Delta_1=0{\cdot}55\pm0{\cdot}10$ (extrapolating slightly the apparent decrease in estimates with increasing order), $\mu_{2,0}=2{\cdot}6\pm0{\cdot}1$ and $\mu_{2,1}=1{\cdot}3\pm0{\cdot}1$. These values compare favourably with those above from Baker–Hunter analysis.

5.3.1. *Analysis of the crossover function.* The crossover function, defined in equation (7), describes the effect of small exchange anisotropy on the scaling functions. This is discussed in considerable detail by Pfeuty *et al* (1974). These authors presented eighth-order series from which one can infer eighth-order series for the axial-anisotropy crossover function on the FCC net. Using completely general results for the tenth-order susceptibility series in the presence of both or either rhombic and axial

Table 5. Padé-approximant analysis of the Baker–Hunter transformation of the series for the reduced second moment, μ_2/χ, of the $S=\infty$ Heisenberg model. The estimate $K_c(\infty)=0{\cdot}31491$ is employed in the transformation. The Padé tables for 2ν, Δ_1, $\mu_{2,0}$, and $\mu_{2,1}$ are given sequentially.

2ν

M \ N	2	3	4	5	6	7
2	1·437	1·413	1·433	1·452	1·439	1·438
3	1·422	1·433	1·444	1·444	1·438	
4	1·371	1·453	1·444	1·444		
5	1·431	1·439	1·438			
6	1·432	1·438				
7	1·436					

Δ_1

M \ N	2	3	4	5	6	7
2	0·67	—	0·69	0·53	0·83	—
3	0·82	0·69	0·61	0·61	—	
4	—	0·52	0·61	0·61		
5	—	0·75	0·86			
6	—	0·81				
7	0·70					

$\mu_{2,0}$

M \ N	2	3	4	5	6	7
2	2·88	3·20	2·93	2·65	2·86	2·88
3	3·06	2·92	2·78	2·78	2·88	
4	3·39	2·64	2·78	2·78		
5	2·99	2·86	2·88			
6	2·96	2·87				
7	2·91					

$\mu_{2,1}$

M \ N	2	3	4	5	6	7
2	1·18	—	1·15	1·24	3·72	—
3	1·23	1·14	1·23	1·23	—	
4	—	1·23	1·23	1·23		
5	—	1·75	3·49			
6	—	2·29				
7	0·43					

Table 6. As in table 5 except that $K_c(\infty)=0{\cdot}31496$, rather than $K_c(\infty)=0{\cdot}31491$ is employed in the Baker–Hunter transformation. In the [4/5] approximant there are two secondary poles with $\Delta_1=0{\cdot}36$ and $0{\cdot}73$.

2ν

M \ N	2	3	4	5	6	7
2	1·439	1·417	1·436	1·462	1·452	1·468
3	1·425	1·436	1·449	1·455	1·457	
4	1·371	1·463	1·455	1·464		
5	1·436	1·452	1·457			
6	1·435	1·471				
7	1·451					

Δ_1

M \ N	2	3	4	5	6	7
2	0·67	—	0·69	0·50	0·60	0·39
3	0·80	0·68	0·60	0·56	0·53	
4	—	0·49	0·56	0·36		
5	—	0·60	0·53			
6	—	0·34				
7	—					

$\mu_{2,0}$

M \ N	2	3	4	5	6	7
2	2·86	3·15	2·90	2·53	2·69	2·38
3	3·03	2·89	2·72	2·64	2·61	
4	3·39	2·51	2·64	2·44		
5	2·93	2·69	2·61			
6	2·94	2·30				
7	—					

$\mu_{2,1}$

M \ N	2	3	4	5	6	7
2	1·20	—	1·17	1·34	1·33	1·21
3	1·23	1·17	1·28	1·31	1·30	
4	—	1·33	1·31	0·81		
5	—	1·41	1·30			
6	—	1·23				
7	—					

Table 7. Four-fit analysis of $\mu_2(\infty)/\chi(\infty)$ using $K_c(\infty)=0\cdot31496$, as in table 6.

N	2ν	Δ_1	$\mu_{2,0}$	$\mu_{2,1}$
7	1·444	0·62	2·78	1·23
8	1·450	0·59	2·71	1·27
9	1·452	0·58	2·69	1·29
10	1·453	0·57	2·67	1·30

anisotropy (Camp and Van Dyke 1974) we have derived tenth-order series for the crossover functions. Herein we have analysed the axial-anisotropy crossover function for which the series coefficients are 0, 4·0, 14·9333333333, 52·5866666667, 179·721481481, 604,358772488, 2011·94011993, 6651·25757867, 21875·0826198, 71658·5001641, and 233999·204149 (to twelve-place accuracy) for orders zero through ten, respectively.

In table 8 the Padé analysis of the Baker–Hunter transformation of $[\chi^{-1}(\partial\chi/\partial g)]_{g=0}$ is presented. The Padé table is quite 'noisy'—evidently the crossover series is more poorly converged than the susceptibility and moment series. There is significant order-to-order variation, as well as differences between the 'corner-of-the-table' and 'centre-of-the-table' estimates. The estimates for Δ_1 are low, and apparently rising with increasing order toward $\Delta_1=0\cdot5\pm0\cdot1$. The crossover-exponent estimates are consistent with the estimate $\phi=1\cdot30\pm0\cdot02$. We may roughly estimate that the amplitudes $X_{0,g}$ and $X_{1,g}$ are, respectively, $2\cdot8\pm0\cdot3$ and $1\cdot2\pm0\cdot3$.

We can circumvent the problem of choosing $K_c(\infty)$ by analysing the 'renormalized' series obtained by dividing the series coefficients for $[\partial\chi/\partial g]_{g=0}$ *term-by-term* by those for $\chi(\infty)$. This series has critical point at $K_c=1\cdot0$ with dominant exponent $\gamma+\phi+1-\gamma=1+\phi$ (Pfeuty *et al* 1974). Further, if $[\partial\chi/\partial g]_{g=0}$ and $\chi(\infty)$ have confluent secondary poles with exponents $\gamma-\Delta_1$ and $\gamma+\phi-\Delta_1$, respectively, the renormalized series has a secondary pole at $K_c=1\cdot0$ with exponent $\phi+1-\Delta_1$. We have studied the renormalized series for axial anisotropy. To twelve-place accuracy the first eleven series coefficients are 0·0, 1·0, 2·10909090909, 3·30515463918, 4·57260501411, 5·90182303221, 7·28551198337, 8·71806796502, 10·1952089680, 11·7135278387, and 13·2701985709.

The analysis of the Baker–Hunter transformation (with, exactly, $K_c=1$) of the renormalized series for ϕ is given in table 9. The Padé table is strikingly better than that in table 8. Here one would estimate $\phi=1\cdot31^{+0\cdot02}_{-0\cdot03}$ and $\Delta_1=0\cdot47^{+0\cdot14}_{-0\cdot06}$. However, it is worth noting that those approximants which reproduce the best estimate $\Delta_1\simeq0\cdot54$ from analysis of $\chi(\infty)$ and $\hat{\mu}_2(\infty)$ yield consistently estimates for ϕ in the range $\phi\approx1\cdot28$–$1\cdot29$. All the approximants with $\phi<1\cdot25$ should probably be disregarded since they do not reproduce a secondary pole.

In summary, although the series is not well behaved, we are able to estimate that the crossover exponent ϕ is in the range $\phi\simeq1\cdot28$–$1\cdot32$ and that the correction exponent lies in the range $\Delta_1\approx0\cdot47$ ($\phi=1\cdot32$)–$0\cdot55$ ($\phi=1\cdot28$). The estimate for ϕ in particular is considerably different from previous series estimates, $\phi=1\cdot25$ (Pfeuty *et al* 1974) and $\phi=1\cdot263$ (Camp and Van Dyke 1974). At present we do not know how much of this difference is real—i.e., due to corrections not taken into account in previous analyses—and how much is due to the poor behaviour of the series. We plan in a later publication (Camp and Van Dyke 1975b) to take up the full question of two-parameter

Table 8. Padé-approximant analysis of the Baker–Hunter transformed series for $[\chi^{-1}\,\partial\chi/\partial g]_{g=0}$. The critical point is assumed to be $K_c(\infty)=0{\cdot}31491$.

ϕ

M \ N	2	3	4	5	6	7
2	1·335	1·226	1·396	1·260	1·272	1·274
3	1·204	1·405	1·283	1·320	1·305	
4	1·277	1·262	1·321	1·308		
5	1·283	1·275	1·305			
6	1·273	1·279				
7	1·332					

Δ_1

M \ N	2	3	4	5	6	7
2	0·32	0·86	0·31	—	—	—
3	—	0·31	0·55	0·36	0·43	
4	—	—	0·36	0·41		
5	—	0·81	0·43			
6	—	—				
7	—					

$x_{0,g}$

M \ N	2	3	4	5	6	7
2	2·25	3·73	1·44	3·59	3·43	3·41
3	3·76	1·34	3·21	2·54	2·83	
4	3·35	3·56	2·52	2·79		
5	3·29	3·38	2·84			
6	3·41	3·32				
7	2·52					

$X_{1,g}$

M \ N	2	3	4	5	6	7
2	1·68	0·25	2·48	—	—	—
3	—	2·58	0·79	1·40	1·16	
4	—	—	1·43	1·18		
5	—	0·78	1·16			
6	—	—				
7	—					

Table 9. Padé-approximant analysis of the Baker–Hunter transformed, renormalized series for the crossover exponent, ϕ. The exact critical point $K_c = 1{\cdot}0$ is employed.

ϕ						
M \ N	2	3	4	5	6	7
2	1·379	1·335	1·269	1·287	1·380	1·184
3	1·288	1·269	1·320	1·319	1·309	
4	1·274	1·287	1·319	1·320		
5	1·137	1·382	1·309			
6	1·287	1·192				
7	1·248					

Δ_1						
M \ N	2	3	4	5	6	7
2	0·45	0·46	0·61	0·53	0·40	—
3	0·52	0·61	0·46	0·47	0·48	
4	0·57	0·53	0·47	0·46		
5	—	0·40	0·48			
6	0·70	—				
7	—					

anisotropy crossover scaling in the spin-infinity Heisenberg susceptibility and correlation function. The question of corrections to scaling will also be dealt with more thoroughly therein.

6. Summary

Confluent corrections to scaling are an important effect in the spin-infinity Heisenberg model, but apparently are absent at $S=\frac{1}{2}$. In this respect the Heisenberg model mirrors the behaviour of the spin-S Ising model for which the amplitude of corrections to scaling decreases continuously with decreasing S, and apparently vanish at $S=\frac{1}{2}$ (*Saul et al* 1975, Camp and Van Dyke 1975a, Camp *et al* 1975). However, the Heisenberg series are not as 'clean' as those of the Ising model. In particular non-confluent corrections are apparently much more important (especially at $S=\frac{1}{2}$) than in the Ising model. Thus although the 'best' estimates $\gamma(\frac{1}{2}) = 1{\cdot}42\text{–}1{\cdot}44$ and $\gamma(\infty) = 1{\cdot}41\text{–}1{\cdot}44$ for the susceptibility exponents closely overlap, the scatter, in $\gamma(\frac{1}{2})$ particularly, is so great that we can only claim that inclusion of confluent corrections in $\chi(\infty)$ leads to exponents $\gamma(\frac{1}{2})$ and $\gamma(\infty)$ which are *probably* consistent with universality. Further work on the possibility of non-confluent corrections is called for, although the prospects for success are rather poor using ill behaved ninth-order series. Perhaps renormalization-group methods can be used to investigate the effect of other competing fixed points, which can be shown to lead to non-confluent singularities. In this regard, it is perhaps worth noting that the relative stability of the cubic fixed point and the Heisenberg fixed point has not been completely resolved (Aharony and Bruce 1974).

The correction exponent $\Delta_1 = 0{\cdot}54 \pm 0{\cdot}10$ is consistently reproduced in all three $S=\infty$ functions analysed: $\chi(\infty)$, $\hat{\mu}_2(\infty)$ and $\chi(\infty)^{-1}[\partial\chi(\infty)/\partial g]_{g=0}$. The 'best' previous $S=\infty$ estimate $\nu \simeq 0{\cdot}717 \pm 0{\cdot}008$ (Ferer *et al* 1971) for the correlation-length exponent is in good agreement with the value $\nu \simeq 0{\cdot}725 \pm 0{\cdot}015$ estimated herein. However, the previous estimates $\phi \simeq 1{\cdot}25$–$1{\cdot}26$ (Pfeuty *et al* 1974, Camp and Van Dyke 1974) are considerably lower than our central estimate $\phi = 1{\cdot}30 \pm 0{\cdot}03$.

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