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LETTER TO THE EDITOR

# Confluent singularities and hyperscaling in the spin-$\frac{1}{2}$ Ising model

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**Abstract.** Using a confluent singularity analysis based on the generalised recurrence method, the series for the correlation length in terms of a dimensionless coupling constant is analysed, extending an approach of Nickel and Sharpe. The results suggest that the spin-$\frac{1}{2}$ BCC Ising model satisfies hyperscaling and has the same confluent singularity structure expected for models of the ($n = 1$, $d = 3$) universality class.

A long-standing puzzle in the theory of critical phenomena has been the apparent failure of hyperscaling in the three-dimensional spin-$\frac{1}{2}$ Ising model (Baker 1977, Baker and Kincaid 1979). The apparent absence (Sykes *et al* 1972, Saul *et al* 1975, Camp and Van Dyke 1975, Camp *et al* 1976) of the confluent singularities originally suggested by Wortis (1970) and predicted by renormalisation group theory (Wegner 1972) has also been puzzling . The purpose of this letter is to present new evidence which points toward a resolution of one or both of these questions.

Following a recent re-examination of the hyperscaling question by Nickel and Sharpe (1979), we have performed a confluent singularity analysis on the series for the correlation length $\xi$ in terms of a dimensionless coupling constant. The results suggest that the BCC spin-$\frac{1}{2}$ Ising model satisfies hyperscaling and, more definitely, exhibits the confluent singularity structure expected of the ($n = 1$, $d = 3$) universality class.

Specifically, our approximants are consistent with hyperscaling and give a value of $3u^*/16\pi \simeq 1{\cdot}43$ for the universal renormalised coupling constant, which is close to that obtained from Callen–Symanzik perturbation theory (Baker *et al* 1978). The first correction to the scaling exponent is estimated to be $\omega_1 \simeq 0{\cdot}79$, in good agreement with results for the continuum model (Baker *et al* 1978); thus, the Wortis–Wegner correction to the scaling exponent is $\Delta_1 = \omega_1\nu \simeq 0{\cdot}50$ ($\nu \simeq 0{\cdot}63$). We also report for the first time from series analysis an estimate for the second correction to the scaling exponent, $\omega_2 \simeq 1{\cdot}4$, which appears to be distinct from $2\omega_1$; this value is in rough agreement with a preliminary result of the scaling field approach (Golner and Riedel 1976, Reidel *et al* 1979, unpublished).

As in the argument of Nickel and Sharpe, it is convenient to examine the series for $x(y) \equiv (\xi/a)^2$ in terms of a dimensionless variable $y$ which varies linearly with $x$ for small $x$. This variable is directly related to the renormalised coupling constant $u$; for the BCC lattice, $3u/16\pi = (1/2\pi\sqrt{3})y^{-3/2}$. The series $x(y)$ is obtained by reverting high temperature series for the susceptibility $\chi$, for the second moment of the spin–spin correlation function $M_2$, and for the fourth field derivative of the free energy $\partial^2\chi/\partial H^2$, using the definitions $\xi^2 \sim M_2/\chi$ and $u \sim \xi^{-d}(\partial^2\chi/\partial H^2)/\chi^2$.

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From a generalised scaling theory which permits violations of hyperscaling (see, for example, Fisher 1973) one expects a leading behaviour for $y$ of the form

$$y \underset{x\to\infty}{=} x^{d^*/d}(\mu_0+\mu_1 x^{-\omega_1/2}+\mu_2 x^{-\omega_2/2}+\ldots) \tag{1}$$

where $\omega_i$ are the corrections to scaling exponents (or integral multiples thereof) and $\mu_i$ are smooth functions. The validity of hyperscaling implies that the anomalous dimension $d^*=0$, and hence that $y$ tends to a *finite* critical value $y^*$ as the correlation length diverges. Thus, if hyperscaling holds,

$$x(y)/y \underset{y\to y^*}{=} A_1(1-y/y^*)^{-\lambda_1}+A_2(1-y/y^*)^{-\lambda_2}+\ldots \tag{2}$$

where $\lambda_1=2/\omega_1$, $\lambda_2=(2-\omega_2+\omega_1)/\omega_1$, etc.

Instead of analysing $x(y)$, Nickel and Sharpe examined the series for $\gamma(y)=(\mathrm{dln}\, x/\mathrm{d}y)^{-1}$ by Padé approximant techniques. They concluded with a reasonable degree of confidence that $\gamma(y)$ for the BCC lattice does have a zero at $y^*$, in support of the hyperscaling hypothesis (although an analysis in the temperature plane gave conflicting results). Now it is implicit in such a Padé approximant analysis that $y^*$ is a simple zero of $\gamma(y)$ or that corrections beyond the leading term are weak. However, the presence of a second zero close to $y^*$ in their approximants leads one to conjecture that $y^*$ is the beginning of a branch-point singularity due to the confluent singularity structure in equation (2).

We have therefore performed a confluent singularity analysis on the series expansion $x(y)/y$ using a generalisation of the recurrence method (Guttmann and Joyce 1972). This method is described in detail in a forthcoming article (Rehr *et al* 1979). In brief, the series coefficients in $x(y)/y=\Sigma_0^\infty c_n y^n$ are fitted to the polynomial coefficients of a linear differential equation of order $K$,

$$\sum_{i=0}^{K} Q_i(y)\Delta^i\psi(y)=P(y) \qquad \Delta\equiv y(\mathrm{d}/\mathrm{d}y) \tag{3}$$

where $Q_i(y)$ are polynomials of respective degrees $M_i$ and $P(y)$ is a polynomial of degree $L$. These *differential equation approximants* $[M_0, M_1, \ldots M_K; L]$ represent a natural generalisation of the Padé approximant; for example, the Dlog Padé approximant corresponds to a first-order, homogeneous differential equation of the form (3). The singular points of each approximant are given by the zeros of the polynomial $Q_K(y)$, and the critical exponents are determined from the solution of the *indicial equation* at these points (see, for example, Ince 1927). To represent a function with two confluent power-law singularities, approximants of second or higher order are required; also in this case $Q_K(y)$ must have a double zero at $y^*$, though good estimates of the critical exponents are possible if two zeros of $Q_K$ are sufficiently close.

We examined first homogeneous $[M_0, M_1, M_2]\equiv[M_0, M_1, M_2; \phi]$ approximants. These approximants *all* exhibited singularities at $y^*\simeq 0{\cdot}160$. This is consistent with a conclusion that $d^*=0$, but since $d^*$ could be very small, this conclusion cannot be made with certainty. Biased estimates of the critical parameters in equation (2) were then made by fixing $y^*$ to be a double zero of $Q_K(y)$ for several values of $y^*$ close to $0{\cdot}160$. It has been observed (Rehr *et al* 1979) from test series that this is a reliable method of estimating the correct critical parameters when the exact critical-point location is not known.

The conjecture that $y^*$ is a confluent singularity point of $x(y)$ is borne out by the observation that the singularity structure of the $[M_0, M_1, M_2]$ approximants in the $y$ plane is stable if $y^*$ is a double zero of $Q_2(y)$. The pair of characteristic BCC singularities (Gaunt and Guttmann 1974) at $\sim\pm 120°$ found in many approximants are outside the circle of convergence $|y| = y^*$, and no other singularities are nearby when $M_2 > 4$. Also, the approximants examined yielded reasonably consistent estimates for the two critical exponents $\lambda_1$ and $\lambda_2$.

Our results for these exponents at $y^* = 0{\cdot}1602$, a value of minimal scatter among the various approximants, are given in table 1. Note that the scatter among the estimates of the dominant exponent is larger than that for the leading correction term. This is unusual in our experience and is due to the smallness of the critical amplitude $A_1$. From these approximants we estimate that $\lambda_1 \simeq 2{\cdot}53$ and $\lambda_2 \simeq 1{\cdot}74$, both with uncertainty of a few per cent. Related quantities are listed in table 2.

**Table 1.** Critical exponents $\lambda_1$ and $\lambda_2$ from $[M_0, M_1, M_2]$ approximants at $y^* = 0{\cdot}1602$.

| $M_0, M_1$ \ $M_2$ | 3 | 4 | 5 | 6 |
|---|---|---|---|---|
| 3, 3 | 2·555 | 3·017 | 1·796 | 3·025 |
| | 1·706 | 1·733 | 1·580 | 1·770 |
| 4, 4 | 1·790 | 2·554 | 2·433 | 2·538 |
| | 1·172 | 1·767 | 1·761 | 1·769 |
| 5, 5 | 1·788 | 2·519 | | |
| | −0·476 | 1·763 | | |

**Table 2.** Critical parameters for the BCC, $s = \frac{1}{2}$ Ising model derived from $y^* = 0{\cdot}1602$, $\lambda_1 = 2{\cdot}53$, $\lambda_2 = 1{\cdot}74$ (see text) and (in parentheses) results from other work.

| | |
|---|---|
| $3u^*/16\pi$ | 1·433 (1·416[a]) |
| $\omega_1$ | 0·79 (0·788[a]) |
| $\Delta_1$ | 0·50 (0·496[a]) |
| $\omega_2$ | 1·4 (1·5[b]) |
| $\Delta_2$ | 0·90 |

[a] Baker *et al* (1978); [b] Riedel *et al* (1979, unpublished).

Although $y^*$ is a singular point of the differential equation approximants, the corresponding solutions are unphysical *unless* $x(y) = (\xi/a)^2$ is positive over the full physical range $0 \leqslant y \leqslant y^*$. The possibility of $x$ dropping below zero might be interpreted as an indication of the failure of hyperscaling, as the zero at $y^*$ has been built into our biased analysis. To check this possibility we have integrated the [4, 4, 4] approximant numerically, thereby obtaining the *integral approximant* for $x(y)/y$ (Hunter and Baker 1979; see also Fisher and Au-Yang 1979, Rehr *et al* 1979). Defining an effective exponent $\lambda(\omega) = \mathrm{d}\ln(x/y)/\mathrm{d}\omega$ with $\omega \equiv -\ln(1 - y/y^*)$, one finds from equation (3) with $P = 0$ that $\lambda(\omega)$ satisfies a nonlinear, first-order differential equation

$$R_2(\mathrm{d}\lambda/\mathrm{d}\omega) + R_2\lambda^2 + R_1\lambda + R_0 = 0 \qquad (4)$$

where $R_0 = Q_0$, $R_1 = y(Q_1 + Q_2)/(y^* - y) + R_2$ and $R_2 = y^2Q_2/(y^* - y)^2$. We remark that $R_i(y)$ are the coefficients in a differential equation for $x(y)/y$ similar to (3) but with the origin shifted to $y^*$. Note that the fixed points of equation (4) are the solutions of the indicial equation at $y^*$; i.e. $\lambda = \lambda_1$ (stable) and $\lambda = \lambda_2$ (unstable).

A difficulty with this calculation stems from the fact that $y = 0$ is a regular singular point of equation (3), so that an integration beginning at $\omega = 0$ is unstable. We have therefore used as an initial condition the value of $\lambda(\omega)$ at $\omega = 0{\cdot}15$; this value correct to ten significant figures was determined from the series expansion for $x(y)$. The integration was then performed using a four-point Runge–Kutta–Gill algorithm, with a step size $0{\cdot}0005$ for $\omega \leq 1$. The results are plotted in figure 1. The critical amplitude $A_1 \simeq +0{\cdot}0087$ was evaluated by Simpson's rule using

$$A_1 = y^* \exp\left(\int_0^\infty (\lambda(\omega) - \lambda_1)\,\mathrm{d}\omega\right). \tag{5}$$

The amplitude $A_2 \simeq +0{\cdot}30$ was then estimated from the expression

$$A_2/A_1 = \lim_{\omega\to\infty} \frac{\lambda_1 - \lambda(\omega)}{\lambda(\omega) - \lambda_2} \exp[(\lambda_1 - \lambda_2)\omega]. \tag{6}$$

Due to the sensitivity of the calculations on the integration procedure, the values of $A_1$ and $A_2$ reported here must be regarded as tentative. The value of $A_1$ is several times larger than that corresponding to the error bounds on the null results for confluent singularities in $\chi$ (Camp *et al* 1976). The result that *both* critical amplitudes are positive lends added support to the validity of hyperscaling. However, due to the smallness of $A_1$, this result must be viewed cautiously. If $A_1$ were slightly negative, the opposite conclusion might be drawn. These results imply that *at least* one of the series

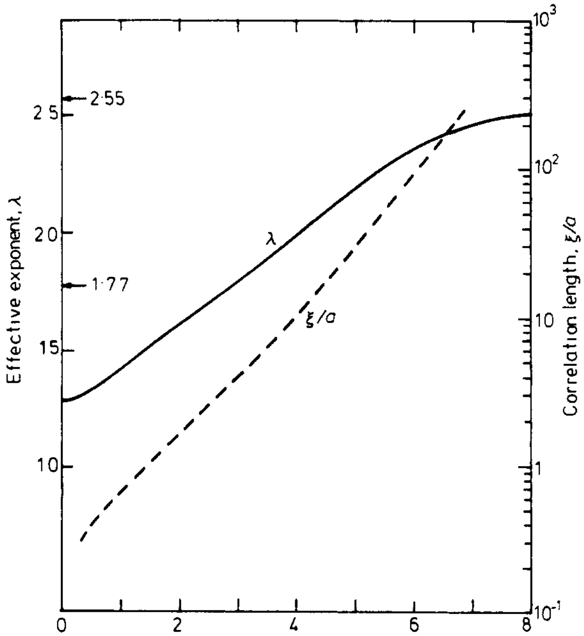


**Figure 1.** Effective exponent $\lambda = \mathrm{d}\ln(x/y)\,\mathrm{d}\omega$ against $\omega = -\ln(1 - y/y^*)$ obtained by integrating the [4, 4, 4] approximant ($\lambda_1 \simeq 2{\cdot}554$, $\lambda_2 \simeq 1{\cdot}767$). Also shown is the correlation length $\xi = ax^{1/2}$, units of the lattice constant $a$.

$\chi$, $M_2$, or $\partial^2\chi/\partial H^2$ should have contributions from the leading confluent correction term and that the second confluent correction to the scaling term should be present with appreciable magnitude. A possible explanation of why such terms have not been apparent in previous temperature-plane analyses is that $\Delta_2 = \omega_2\nu \simeq 0{\cdot}9$ is very close to unity, and probably indistinguishable from observed analytical factors. In summary, we have found additional evidence for the validity of hyperscaling in the BCC, $s = \frac{1}{2}$ Ising model. However, whether hyperscaling is valid or not, the leading confluent singularity structure is found to be consistent with that of the $(n = 1, d = 3)$ universality class.

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