

Comment on “Reconciliation of high-temperature series and renormalization-group results by suppressing confluent singularities”

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We have used a slightly modified version of Roskies’s quadratic map method [Phys. Rev. B **24**, 5305 (1981)] to estimate the confluent correction amplitudes for the susceptibility χ and correlation length ξ of a model that interpolates between Ising and Gaussian limits. Our best estimates for the corresponding leading exponents are $\gamma=1.237\pm 0.003$, $\nu=0.630\pm 0.003$, and $\eta=2-\gamma/\nu=0.036\pm 0.002$. The correction to scaling amplitude ratio $B(\xi)/B(\chi)=0.8\pm 0.1$ is slightly larger than that predicted from ϕ^4 continuum model analysis [M.-c. Chang and A. Houghton, Phys. Rev. Lett. **44**, 785 (1980) and C. Bagnuls and C. Bervillier, Phys. Rev. B **24**, 1226 (1981)].

Roskies has described recently¹ a simple procedure for obtaining critical exponent estimates from high-temperature series on the assumption that the leading correction to scaling exponent θ is precisely 0.5 and that higher-order corrections, including possible analytic background terms, are negligible. The key idea is to eliminate the confluent corrections by a quadratic mapping; we use

$$1-x=p^2(1-z)^2/(p-z)^2, \tag{1}$$

where x is either the normalized inverse-temperature K/K_c or the related v/v_c with $v=\tanh K$. The relation (1) maps the critical point $K=K_c$ onto $z=1$ independent of the parameter p and with $2\sqrt{2}-1\leq p\leq\sqrt{2}+1$ this mapping is in the acceptable region established by Roskies.¹ Furthermore, we follow Roskies’s prescription for the loose-packed lattices which is to map the anti-ferromagnetic singularity at $x=-1$, $z=-(\sqrt{2}-1)p/(p-\sqrt{2})$ as far from the origin as the possible singularity at $x=\infty$, $z=p$. This requires

$$p=2\sqrt{2}-1. \tag{2}$$

Our method differs from that described by Roskies only in that we do not impose *a priori* a critical point location but rather adjust K_c or v_c until the Dlog Padé approximants in the z plane are singular at precisely the expected critical point $z=1$.

We have applied the method to what is appropriately described as a double-Gaussian model.

The model as a function of inverse temperature K and magnetic field h is defined by the partition function

$$Z = \prod_i \left[\int dS_i f(S_i) \right] \times \exp \left[K \sum_{nn} S_i S_j + h \sum_i S_i \right], \tag{3}$$

where the spin distribution on each lattice site i is

$$f(S) = \exp[-(S-\sqrt{y})^2/2w^2] + \exp[-(S+\sqrt{y})^2/2w^2], \tag{4}$$

$$y=1-w^2.$$

The second moment of this distribution is identically unity and the width w or related parameter y enables one to interpolate between Ising ($y=1$) and Gaussian ($y=0$) limits. High-temperature series for the zero-field susceptibility $\chi = \sum_i \langle S_o S_i \rangle$ and correlation length squared $\xi^2 = \sum_i r_{oi}^2 \langle S_o S_i \rangle / \chi$ have been derived to order K^{21} on the bcc lattice² and will be reported elsewhere.³ The general coefficient of K^n in these series is a polynomial in y of degree approximately n so that the series can be analyzed by two variable approximant methods.⁴ However, here we restrict ourselves to analyzing a single-variable series in K with y fixed at the discrete values $y=1.0, 0.95, 0.9, \dots, 0.6$. For $y\leq 0.6$ the leading correction to scaling amplitude is so large that the neglect of higher-order correc-

tions is probably not justified.

The results described below were obtained by standard *Dlog Padé* analysis of z plane series for χ , $K\chi$, ξ^2 , and ξ^2/K supplemented by a Newton-Raphson search for K_c to yield a pole at $z=1$. If the K plane function that is transformed via (1) and (2) has the expected critical behavior

$$F(K) \approx A(1-K/K_c)^{-\lambda} \times [1 + B(1-K/K_c)^\theta + \dots],$$

$$\theta = 0.5,$$
(5)

then from the residue at $z=1$ we obtain the exponent λ and from the background the amplitude B . We find the exponents $\lambda = \gamma$ or 2ν remarkably independent of y , that is, universal. We also find the strong correlations between λ and B shown in Fig. 1 just as expected on the basis of simple ratio analysis.² Finally, we note that the χ and ξ^2 exponents must be strongly correlated if we accept the universality hypothesis that the correction to scaling amplitudes vanish at the same y value for both functions. With our preferred estimates $\gamma = 1.237$ and $\nu = 0.630$, this special $y = 0.85$. Also, this choice yields $\eta = 2 - \gamma/\nu = 0.0365 \pm 0.0015$. Our analysis appears to be consistent in that if we impose no conditions on the amplitudes but demand instead that the χ and ξ^2 series diverge at the same K_c , we obtain $\eta = 0.0357 \pm 0.0015$. For the spin- $\frac{1}{2}$ model, i.e., $y=1$, our preferred estimates $\gamma = 1.237$ and $\nu = 0.630$ correspond to a critical $v_c = \tanh K_c \approx 0.156086$, whereas the choice $\gamma = 1.240$ corresponds to $v_c \approx 0.156090$ in agreement with Roskies.¹

As a further test of universality and/or analysis consistency we show the differential ratio of the correction to scaling amplitudes in Fig. 2. This ratio varies by order 20% which is well outside the apparent uncertainties one would have guessed from the data of Fig. 1. The most likely explanation is that either the bias $\theta = 0.5$ or the neglect of higher-order corrections have resulted in an "effective" but otherwise spurious fit for both the amplitudes and, to a lesser extent, the exponents γ and ν . The quadratic mapping by itself does not allow one to estimate the magnitude of these effects and thus the present calculation can serve principally as a benchmark for other analyses^{3,4} in which more degrees of freedom are allowed in the fits.

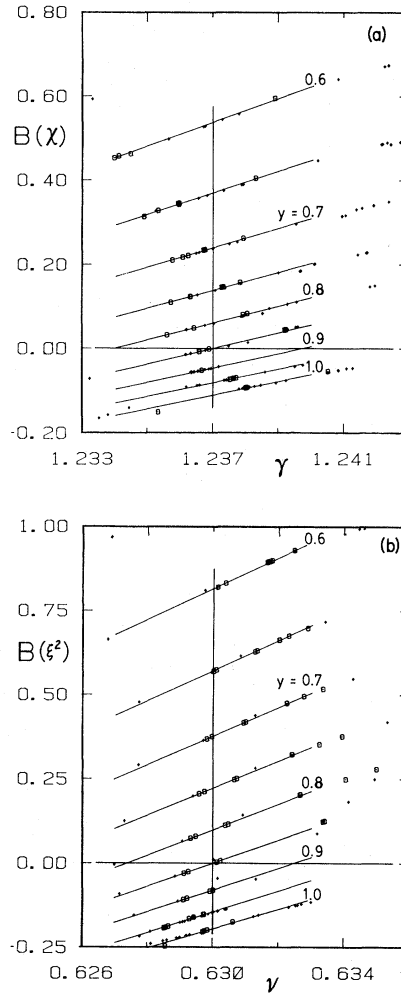


FIG. 1. Correlation plots of correction to scaling amplitude vs leading exponent from near diagonal *Dlog Padé* estimates based on series of order 18–21. Estimates based on the full 21 term series are circled. Solid lines are drawn as a guide to the eye in the most probable range $\gamma = 1.237 \pm 0.003$ and $\nu = 0.630 \pm 0.003$.

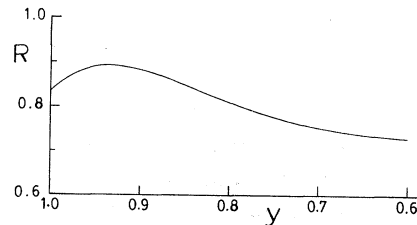


FIG. 2. Differential amplitude ratio $R = (dB(\xi)/dy)/(dB(\chi)/dy)$ vs double-Gaussian model parameter γ . Amplitude estimates come from the solid-line intersections shown in Fig. 1 at the exponent values $\gamma = 1.237$ and $\nu = 0.630$.

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¹R. Z. Roskies, *Phys. Rev. B* **24**, 5305 (1981).

²B. G. Nickel, in *Phase Transitions: Cargèse 1980*, edited by M. Levy, J.-C. Le Guillou, and J. Zinn-Justin (Plenum, New York, 1982), pp. 291–324.

³B. G. Nickel and J. J. Rehr (unpublished).

⁴M. E. Fisher, in *Statistical Mechanics and Statistical Methods in Theory and Application*, edited by U.

Landman (Plenum, New York, 1977), pp. 3–32; J.

-H. Chen, M. E. Fisher, and B. G. Nickel, *Phys. Rev. Lett.* **48**, 630 (1982).