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Two-Series Approach to Partial Differential Approximants: Three-Dimensional Ising Models

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A two-series approach to partial differential approximant analysis of power series is presented. Instead of double series, $f(x,y)=\sum c_{ij}x^iy^j$, our approach uses two one-variable series in x, f and $\partial f/\partial y$, and has the efficiency and stability of one-variable methods. 21-term high-temperature series are analyzed for the susceptibility and correlation length squared for double-Gaussian Ising models on the bcc lattice. Critical exponents are $\gamma=1.2378(6)$, $2\nu=1.2623(6)$, and $\eta=0.0375(5)$; correction-to-scaling exponents are $\theta_\chi=0.52(3)$ and $\theta_{\xi^2}=0.49(4)$; and the subdominant critical amplitude ratio is $a_\xi/a_\chi=0.83(5)$.

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Partial differential approximants (PDA's) have proved valuable as a method of series analysis in critical phenomena.[1] This approach permits the direct computation of critical exponents and confluent singularities in singular thermodynamic functions of two variables. In addition the scaling function, critical amplitudes, analytic factors, and background terms can be obtained. For a general discussion see the review by Fisher and Chen,[2] and references therein.

The standard PDA method is designed explicitly for the analysis of double power series,

$$f(x,y)=\sum c_{ij}x^iy^i \quad (i\leq N,\ j\leq N'), \tag{1}$$

where N' is typically $O(N)$. For definiteness, we shall consider x to be a high-temperature variable ($x=J/kT$, where J is the Ising nearest-neighbor coupling constant, k is Boltzmann's constant, and T is the temperature) and y to be some irrelevant variable. Briefly, a partial differential approximant to f is a function $F_{[M_1,M_2;L/M_0]}$ which satisfies a partial differential equation of the form

$$P_1\,\partial_xF+P_2\,\partial_yF+P_0F=P_L \tag{2}$$

(where the operator ∂_x is either $\partial/\partial x$ or $x\,\partial/\partial x$) and which reproduces the known terms in the series expansion of f. The quantities $P_i=\sum P_{ij}(y)x^j$ and $P_L=\sum P_{Lj}(y)x^j$ are polynomials specified by the labels M_i and L, respectively. The method of Fisher based on double series has the advantage that all the known series information is used in constructing approximants. A drawback is that the method is computationally time consuming for large N, typically involving the inversion of $NN'\times NN'$ matrices [i.e., $O((NN')^3)$ time steps].

In this paper we present an alternative approach to PDA analysis based, instead of Eq. (1), on two single-variable power series,

$$f(x,y)=\sum_{n=0}c_n(y)x^n \quad (n\leq N) \tag{3}$$

and

$$\frac{\partial f(x,y)}{\partial y}=\sum_{n=0}\frac{\partial c_n(y)}{\partial y}x^n \quad (n\leq N). \tag{4}$$

The leading N terms in f and $\partial f/\partial y$ are considered to be known functions of y which need not be polynomials. The label M_i for any function P_i in Eq.

(2) now represents an integer specifying the degree of P_i as a polynomial in x. Also, the polynomial coefficients, P_{ij}, are not assumed to be polynomials in y, and can be more general functions of y. Given a set of integers defining a given PDA of this type, $[M_1,M_2;L/M_0]$, one can construct the polynomial coefficients P_{ij} and P_{Lj} by matrix inversion of a set of linear equations. For the operator $\partial_x = x\,\partial/\partial x$, these linear equations take the form

$$\sum_0^M\{[(P_{0j}+P_{1j}(n-j)]a_{n-j}+P_{2j}\,\partial_y a_{n-j}\} = P_{Ln}, \quad (0\leq n\leq N), \tag{5}$$

normalized with $P_{10}=1$. At a fixed value of y, one obtains a PDA along a vertical cut, rather than over the x-y plane. The procedure is then repeated at discrete points in the y direction to map out the approximant more completely. This method represents a substantial simplification over the conventional approach in that the size of the matrices that must be solved are only of order $N\times N$, which reduces inversion time requirements by a factor of order N'^3. Thus the method has the simplicity of one-variable methods such as the Padé approximant[3] and (ordinary) differential approximants (DA's).[4,5] An advantage of PDA's over the ordinary differential approximants is the ability to analyze the full scaling function. A DA can analyze only the leading correction-to-scaling term and analytic corrections. Our investigation indicates that the two-series method also has substantially greater ability than does the conventional PDA method and gives results comparable to or better than the best single-variable approaches.

As an initial application we have analyzed Nickel's 21-term high-temperature series for χ and ξ^2/x for the double-Gaussian Ising model on the bcc lattice.[5,6] Here χ is the magnetic susceptibility and $\xi^2 \equiv M_2/\chi$ is the second-moment definition of the correlation-length–squared series. These models are continuous-spin nearest-neighbor Ising models with a spin-weight factor consisting of two identical Gaussians of width $\omega=(1-y)^{1/2}$ at $\pm y$. Chen, Fisher, and Nickel[1] only studied χ with the PDA approach. Since we have analyzed two series with a common scaling behavior, we can also investigate critical amplitude ratios.

We now briefly outline the procedure used to obtain exponents and amplitudes from these approximants. Once an approximant has been calculated by the solution of Eq. (5), the analysis proceeds by determination of the leading positive zeros of the polynomials P_1 and P_2 and the fixed point (or multicritical point), (x^*,y^*), which is a common zero of both polynomials. Next one determines the matrix of partial derivatives $a_{ij} \equiv \partial_j(P_i/P_0)$, $i,j=1,2$ at (x^*,y^*). The derivatives with respect to y must be calculated numerically. Here it is convenient to use the vector notation $\vec{x} \equiv (x,y) \equiv (x_1,x_2)$. Diagonalizing the 2×2 matrix a_{ij}, i.e., solving the eigenvalue problem, $\sum_j a_{ij}\epsilon_{jk}=\lambda_k\epsilon_{ik}$, then yields the critical exponents $\gamma=(\lambda_1)^{-1}$, where λ_1 is the largest positive eigenvalue of a_{ij}, and $\theta=-\lambda_2/\lambda_1$. The eigenvectors ϵ_{ij} define the *linearized scaling fields* appearing in the scaling solution of Eq. (5), $\chi=\chi_0+g_1^{-\gamma}f(g_2/g_1^\theta)$, i.e.,

$$\begin{pmatrix} x-x^* \\ y-y^* \end{pmatrix} = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} \\ \epsilon_{21} & \epsilon_{22} \end{pmatrix}\begin{pmatrix} g_1 \\ g_2 \end{pmatrix}. \tag{6}$$

In our work, the fixed point was located by a Newton-Raphson scheme accurate to within 10^{-6}; convergence was typically achieved within 10 iterations. The partial derivatives with respect to y were calculated by means of a symmetrical, equal-spacing four-point formula with a grid size of $\Delta y=10^{-5}$.

The critical amplitudes and scaling function can be obtained by integration of a given partial differential approximant along a characteristic, i.e., trajectory parametrized by a scalar t. Along this path $dx_i/dt=-a_{ij}(\vec{x}(t))$ and $F(\vec{x}(t))=F(\vec{x}(0))\times e^t$. If the trajectory is sufficiently close to the fixed point, one may simply approximate the function in terms of the linearized scaling fields as

$$F=F_0+g_1^{-\gamma}A_F(1+a_F g_2 g_1^\theta), \tag{7}$$

where F_0 is a background term which is present only for inhomogeneous approximants $(L\geq 0)$. Thus for homogeneous approximants the subdominant amplitude a_F is given by

$$a_F \simeq (g_1^\gamma F)^{-1}\Delta(g_1^\gamma F)/\Delta(g_2 g_1^\theta). \tag{8}$$

For our estimates of a_F, the differences in Eq. (8) were evaluated over an interval of $\Delta x=10^{-4}$ at fixed $y=y^*$ and $x=0.8x^*$. At this value the series representation of f is accurate to approximately 1%.

Our results for the analysis of χ are shown in Fig. 1(a), and those for ξ^2 are shown in Fig. 1(b). The homogeneous approximants used were close to diagonal, typically $M_i=6\pm 2$. There were few well-behaved near-diagonal *inhomogeneous* approximants, none for $L\geq 1$. We also investigated *biased* approximants in which a zero at $-x_c(y)$ was imposed on P_1; this gives rise to an antiferromagnetic fixed point near $(-x^*,y^*)$. Such biasing has little effect on the results for homogeneous approximants [Figs. 1(a) and 1(b)] and permits one to construct many additional approximants. In contrast to

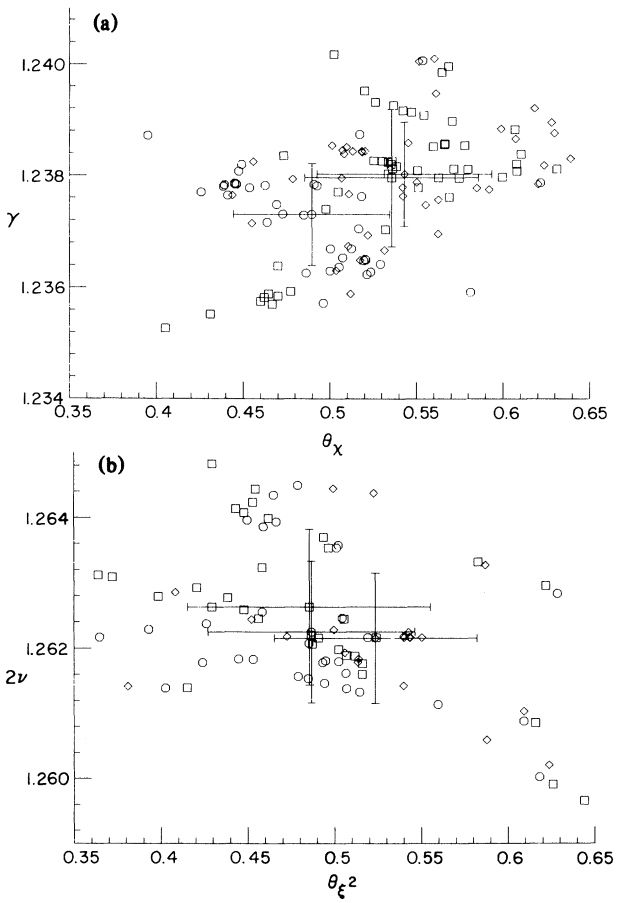

FIG. 1. (a) Susceptibility exponent, γ, and (b) correlation-length–squared exponent, 2ν, vs correction-to-scaling exponent, θ. Homogeneous PDA's are denoted by squares (unbiased) and lozenges (biased); circles denote biased $L=0$ approximants. Centroids and standard deviations are indicated for each type of approximant.

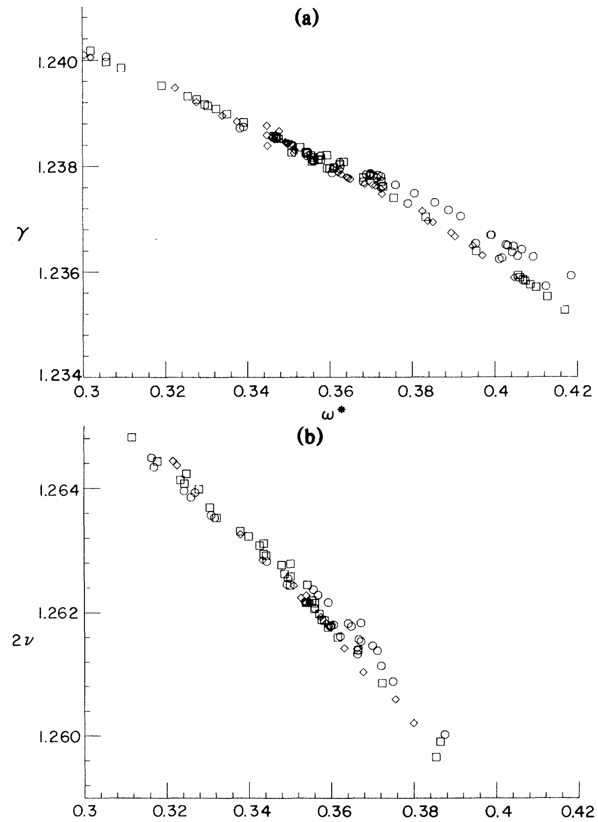

FIG. 2. (a) Susceptibility exponent, γ, and (b) correlation-length–squared exponents, 2ν, vs fixed point estimate, ω^*. Homogeneous PDA's are denoted by squares (unbiased) and lozenges (biased); circles denote biased $L=0$ approximants.

Ref. 1, we did not find that Euler-invariant approximants were special.

Figures 2(a) and 2(b) show the distribution of our approximants with respect to $\omega^* = (1-y^*)^{1/2}$. They show the strong linear correlation of the leading exponent with the location of the fixed pint ω^*. We obtain $y^*_\chi = 0.866(12)$ and $y^*_{\xi^2} = 0.876(6)$. The overall distribution is thus significantly smaller than that of Chen, Fisher, and Nickel,[1] $y^*_\chi = 0.87(4)$. The errors quoted in the present paper refer to 1 standard deviation over the distribution of all approximants within a window of ± 3 standard deviations of the centroid; thus we ignored several spurious approximants outside this window. If we restricted the results to *quartiles* of the distribution of our approximants, in the manner used in Ref. 1, our quoted errors would be even smaller.

A summary of the results for the critical exponents obtained from these approximants is given in Table I, together with a representative sample of results for the 21-term series by other methods of analysis and for the field-theoretic perturbation approach.[7–9]. Results for the correction-to-scaling exponent θ are slightly though not significantly different. Since the correlation of χ and ξ^2 vs y^* is similar, we obtain an estimate for $\eta \equiv 2 - \gamma/\nu$ of 0.0375(5).

Finally we have estimated the amplitude ratios a_ξ/a_χ using Eq. (6). We find that the result is well correlated with y^* and yields 0.83(5), somewhat higher than that from the field-theoretic series results (see Table I).

In conclusion, we have developed an alternative to the conventional PDA analysis method for the analysis of singular functions of two variables. The method has several advantages, including the computational efficiency and simplicity of one-variable

TABLE I. Critical exponents and amplitude ratios for 21-term double-Gaussian and Ising-model susceptibility and correlation-length–squared series with use of partial differential approximants (PDA), ordinary differential approximants (DA), ratio analysis (RA), Padé-Roskies transformation (PR), and field-theoretic analysis (FT).

Analysis	γ	2ν	η	θ	y^*	a_ξ/a_χ	Reference
PDA	1.2378(6)	1.2623(6)	0.0375(5)	0.52(3) (χ) 0.49(4) (ξ)	0.866(12) (χ) 0.876(6) (ξ)	0.83(5)	Present work
PDA	1.2385(15)	⋯	⋯	0.54(5) (χ)	0.87(4) (χ)	⋯	1
DA	1.237(2)	1.260(3)	0.0359(7)	0.51(3)	⋯	0.85	5
PR	1.237(3)	1.260(6)	0.036(2)	⋯	⋯	0.8(1)	10
RA	1.2385(25)	1.261(3)	0.035(3)	⋯	⋯	⋯	11
FT	1.241(2)	1.260(3)	0.031(4)	0.498(2)	⋯	⋯	7
FT	1.241(4)	1.260(4)	0.031(11)	0.496(5)	⋯	⋯	9
FT	⋯	⋯	⋯	⋯	⋯	0.65(5)	8

methods together with increased stability. Also, since a double-power-series representation is not essential, the method extends the class of functions for which PDA's can be constructed. This gives the possibility of new applications; an example is the lattice scalar ϕ^4 model. Both unbiased and biased PDA's can be studied. Our investigation indicated that biasing for an antiferromagnetic singularity may improve stability. A natural generalization of our approach would be to construct approximants along an arbitrary trajectory $[x(t,u),y(t,u)]$, with u fixed, when $x(t,u)$ and $y(t,u)$ are power series in t. Another generalization is to construct approximants based on four series with a common fixed point (x^*,y^*) e.g., χ, $\partial x/\partial y$, ξ^2, and $\partial\xi^2/\partial y$.

An initial application to 21-term, high-temperature double-Gaussian model series was carried out. Only homogeneous and inhomogeneous approximants with a constant driving term $(L=0)$ yielded distributions of approximants with minimal scatter. The results obtained are consistent with the previous analysis of Chen, Fisher, and Nickel, but have significantly less scatter. These results are also, within error bars, consistent with other analyses of the three-dimensional double-Gaussian Ising model series. The results for the dominant critical exponents are slightly higher than the second-order inhomogeneous $(L=1)$ DA results of Nickel and Rehr and slightly lower than the field-theoretic series results. However, both η and the subdominant amplitude ratio a_ξ/a_χ show significant discrepancies with respect to the field-theoretic results.

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

[2]M. E. Fisher and J. H. Chen, in *Phase Transitions,* edited by M. Lévy, J.-C. LeGuillou, and J. Zinn-Justin, NATO Advanced Study Institute Series B, Vol. 72 (Plenum, New York, 1982).

[3]G. A. Baker, Jr., in *The Padé Approximant in Theoretical Physics,* edited by G. A. Baker, Jr., and J. L. Gammel (Academic, New York, 1970).

[4]J. J. Rehr, G. S. Joyce, and A. J. Guttmann, J. Phys. A **13**, 1587 (1980).

[5]B. G. Nickel and J. J. Rehr, unpublished.

[6]B. G. Nickel, in *Phase Transitions,* edited by M. Lévy, J.-C. LeGuillou, and J. Zinn-Justin, NATO Advanced Study Institute Series B, Vol. 72 (Plenum, New York, 1982).

[7]J. C. LeGuillou and J. Zinn-Justin, Phys. Rev. Lett. **39**, 95 (1977), and Phys. Rev. B **21**, 3976 (1980).

[8]C. Bagnuls and C. Bervillier, Phys. Rev. B **24**, 1226 (1981).

[9]G. A. Baker, Jr., B. G. Nickel, and D. I. Meiron, Phys. Rev. B **17**, 1365 (1978).

[10]B. Nickel and M. Dixon, Phys. Rev. B **26**, 3965 (1982).

[11]J. Zinn-Justin, J. Phys. (Paris) **42**, 783 (1981).