Partial Differential Approximants for Multicritical Singularities

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A recently proposed approach—partial differential approximants—for analyzing power series in *two* (or more) variables for functions which exhibit singularities of multicritical, scaling character is tested by analyzing the susceptibility series for the bicritical point describing the Ising-Heisenberg-XY crossover in a three-dimensional classical ferromagnet. Encouraging results are obtained for the unbiased estimation of the bicritical point, of the multicritical exponents γ and ϕ, and of the slopes of the scaling axes.

The method of Padé approximants[1] for analyzing the behavior of a function, $f(x)$, of a single variable x, known only through a finite number of its power-series expansion coefficients, f_j, is justly famous.[2] It has played an especially important role in the study of critical phenomena,[2,3] because of its ability to handle accurately branch-point singularities of the form $f(x)\approx Z_0/(x_c-x)^\gamma$, with nonintegral exponents γ. In particular, by using the D log transformation first introduced by Baker,[4] one can obtain direct, "unbiased," estimates of the critical point x_c and the critical exponent γ; by appropriate further manipulation, the critical amplitude, Z_0, can also be estimated.

In most physical contexts more than one independent variable plays an important role: For example, in the case of a ferromagnet or antiferromagnet one typically has $x=J/k_BT$, with temperature, T, and exchange integral, J, but would also be interested in $y=H/k_BT$, where H is the magnetic field. Physical quantities of interest, like the susceptibility $\chi(T,H)$, will then have expansions in two variables:

$$f(x,y)=\sum_{j,j'=0} f_{jj'}x^jy^{j'}. \tag{1}$$

Given a limited number of coefficients, say $f_{jj'}$ for (j,j') in some label set J, one wants methods for approximating such a function of two variables. Now, the most crucial feature will usually be the expected nature of the singularities of $f(x,y)$. In many cases, particulary in the study of critical and multicritical phenomena,[5-7] there will be a "multisingular point," (x_c,y_c), in the vicinity of which *scaling behavior* is to be anticipated, that is,

$$f(x,y)\approx|\Delta\tilde{x}|^{-\gamma}Z(\Delta\tilde{y}/|\Delta\tilde{x}|^{\phi}), \tag{2}$$

$$\Delta\tilde{x}=\Delta x-\Delta y/e_2,\quad \Delta\tilde{y}=\Delta y-e_1\Delta x, \tag{3}$$

as $\Delta x=(x-x_c)$ and $\Delta y=(y-y_c)\to 0$. Here γ is the exponent scaling f, while ϕ is the crossover exponent; the coefficients e_1 and e_2 specify the slopes of the scaling axes. An *effective* method of approximation should yield estimates for x_c and y_c, for γ and ϕ, for e_1 and e_2, and for the scaling function $Z(z)$, which may *itself* display singularities,[5,6] e.g., of the form $Z(z)\approx\dot{Z}_0|\Delta z|^{-\dot{\gamma}}$ as $\Delta z=z-\dot{z}\to 0$, where $\dot{z}$ is one of a number of possible (scaled) singular points.

An approach has recently been proposed—using "partial differential approximants" (PDA's)—which can, in principle, meet this challenge.[8,9] The purpose of the present Letter is to demonstrate and test this new technique numerically on a realistic, but reasonably well understood, example, namely bicritical crossover in an Ising-Heisenberg-XY model ferromagnet.[6] In fact, the approach is found to perform encouragingly well, so that one may anticipate successful applications to a variety of less well understood physical situations, such as bicriticality in antiferromagnets, tricritical behavior, Potts points, quantal crossover, percolation, etc.

A partial differential approximant $F(x,y)\equiv F_{K;\mathsf{LMN}}(x,y)$ to a function $f(x,y)$, with (partially) given expansion (1), is a solution of the linear partial differential equation[8,9]

$$P_{\mathsf{L}}(x,y)F(x,y)=Q_{\mathsf{M}}(x,y)\frac{\partial F}{\partial x}+R_{\mathsf{N}}(x,y)\frac{\partial F}{\partial y}, \tag{4}$$

whose power series expansion matches that for $f(x,y)$ to at least some determinate low order. The defining equation (4) is specified by three polynomials $P_{\mathsf{L}}=\sum_{l,l'}x^ly^{l'}$, $Q_{\mathsf{M}}=\sum_{m,m'}q_{mm'}x^my^{m'}$, and $R_{\mathsf{N}}=\sum_{n,n'}r_{nn'}x^ny^{n'}$, where the sums run over the assigned label sets $\mathsf{L}\supset(l,l')$, $\mathsf{M}\supset(m,m')$, and $\mathsf{N}\supset(n,n')$ of cardinality $|\mathsf{L}|=L$, $|\mathsf{M}|=M$, and $|\mathsf{N}|=N$. In view of the linearity, the normalization condition $p_{00}\equiv p_{\mathsf{L}}(0,0)$ is usually (but not always) appropriate. The remaining $K=L+M+N-1$ polynomial coefficients, $p_{ll'}$, $q_{mm'}$, and $r_{nn'}$, are to be chosen by replacing $F(x,y)$ in (4) by the given expansion, (1), of $f(x,y)$ and requiring (4) to hold as an identity on all terms $x^k y^{k'}$ with (k,k') in a chosen label set K with $|K|=K$.

This prescription for determining P, Q, and R (for chosen K, L, M, and N) sounds complex but merely leads to a set of K linear algebraic equations which are readily solved by standard computer routines provided they are consistent and nonsingular. As in the determination of ordinary D log Padé approximants (to which the new method, in fact, reduces if one imposes $R=0$ when $y=0$), singular and inconsistent equations can arise; indeed, they are sometimes a sign that $f(x,y)$ satisfies an equation of the form (3) identically![8,9]

An essential feature of a PDA is the following: *If $Q(x,y)$ and $R(x,y)$ have a common zero at (x_0,y_0) then, in the vicinity of this point, the approximant $F(x,y)$ has the scaling form (2) with $\Delta x = x - x_0$ and $\Delta y = y - y_0$.* Thus a common zero, (x_0,y_0), represents an estimate for a multisingular point, (x_c,y_c), of $f(x,y)$. Furthermore, corresponding estimates for the exponents γ and ϕ, and for the axis slopes e_1 and e_2, may be determined explicitly from the approximant polynomials by evaluating $P_0=P(x_0,y_0)$, $Q_1=(\partial Q/\partial x)_0$, $Q_2=(\partial Q/\partial y)_0$, $R_1=(\partial R/\partial x)_0$, and $R_2=(\partial R/\partial y)_0$, where the subscript 0 denotes $x\to x_0$ and $y\to y_0$.

These theoretical conclusions and, in fact, practical numerical results are best obtained by solving the defining PDA equation (4) by the method of characteristics. Thus one introduces a timelike variable τ and the corresponding *ordinary* differential equations

$$dx/d\tau = Q(x,y), \quad dy/d\tau = R(x,y). \tag{5}$$

Given a *trajectory*, $[x(\tau),y(\tau)]$, which solves these equations, one has

$$f(x,y) \simeq F(x,y) = \exp\left[\int^{\tau} P(x(\tau'),y(\tau'))d\tau'\right], \tag{6}$$

where appropriate boundary conditions at $\tau=0$ are understood. This trajectory-integral expression leads[10] to estimates of the scaling function $Z(z)$.

To study the effectiveness of the PDA technique we have considered a classical (spin $S=\infty$), anisotropic, Heisenberg-model ferromagnet on the three-dimensional fcc lattice with nearest-neighbor couplings $J_\perp = J_{xx} = J_{yy} \geq 0$ and $J_\parallel = J_{zz} \geq 0$.[6] We will report, in particular, results for the *total* (reduced) susceptibility $\chi = \chi_\parallel + 2\chi_\perp$, where $\chi_\parallel = k_B T(\partial M_z/\partial H_z)$ and $\chi_\perp = k_B T(\partial M_x/\partial H_x) = k_B T(\partial M_y/\partial H_y)$ while $M_\alpha = \langle s_0{}^\alpha\rangle$ (for $\alpha = x,y,z$).

Now on the basis of renormalization-group analysis[11] and the symmetry properties of $\mathcal{H}$, it is firmly believed that Heisenberg-like critical behavior, with[6] $\gamma \simeq 1.38$, occurs *only* when $J_\perp = J_\parallel$; for $J_\perp < J_\parallel$, Ising-like (or $n=1$) behavior, with exponent[12] $\gamma_I \simeq 1.25$, should occur; conversely, for $J_\perp > J_\parallel$, one expects XY-like (or $n=2$) behavior, with $\gamma_{XY} \simeq 1.31$. With $\bar{J} = \frac{2}{3}J_\perp + \frac{1}{3}J_\parallel$ and $g = (J_\perp - J_\parallel)/\bar{J}$, this means that a multicritical singularity occurs at $g=0$ and $w = \bar{J}/k_B T = w_c$. If this conclusion is granted, the best variables for a series analysis of the multicritical region are[6] w and g ($\simeq 0$). One can then go moderately far by standard, *single*-variable techniques which, in fact, yield[11] $w_c \simeq 0.3147$ and $\phi \simeq 1.25$. In order to *test* the PDA approach, however, we will work with the rather natural variables $x = J_\parallel/k_B T$ and $y = J_\perp/k_B T$. The pure XY and Ising models (for $S=\infty$) then correspond to $x=0$ and $y=0$, respectively, but the multicritical point should be found at $x_c = y_c = w_c$ and the axis slopes should be $e_1 = 1$ ($g=0$) and $e_2 = -\frac{1}{2}$ ($\Delta w = 0$).

Figure 1 is a scatter diagram in the (x,y) plane showing estimates for a range of PDA's using from $|K|=21$ to 36 expansion coefficients for χ (i.e., through orders w^6, w^7, and w^8). The "exact" scaling axes are drawn in the figure. It is remarkable that the estimates tend strongly to lie along a line parallel to (although slightly below) the second scaling axis ($\Delta w = 0$). The precision of these unbiased estimates, which can be gauged by the 0.1% and 1% "boxes," is quite satisfying. (As in standard Padé analysis one would expect improvement by using biased techniques such as the imposition of $x_c = y_c$.) Not surprisingly, better estimates tend to be given when the label sets M and N, for Q and R, match most closely.

A larger region of the (x,y) plane is displayed in Fig. 2, for one of the better approximants (with $|L|=13$, $|M|=|N|=12$). Note the locus of zeros of $Q_M(x,y)$ and $R_N(x,y)$ (dotted curves), whose intersection, $x_0 \simeq 0.3148$ and $y_0 \simeq 0.3151$, locates the estimated multicritical point. The corresponding exponent estimates are $\gamma \simeq 1.398$ and $\phi \simeq 1.282$. The broken straight lines through (x_0, y_0) indicate the corresponding (approximate) scaling axes, with $e_1 \simeq 1.07$ and $e_2 \simeq -0.405$, while the curving lines (dashed and solid) represent trajectories computed from (5). The two solid trajectories originate on the x and y axes at zeros $Q_M(x_I, 0) = 0$ and $R_N(0, y_{XY}) = 0$, which, in fact, yield estimates for the pure Ising and XY critical points. Consequently these trajectories represent estimates of the Ising and XY *critical lines*. It is important to notice that these critical

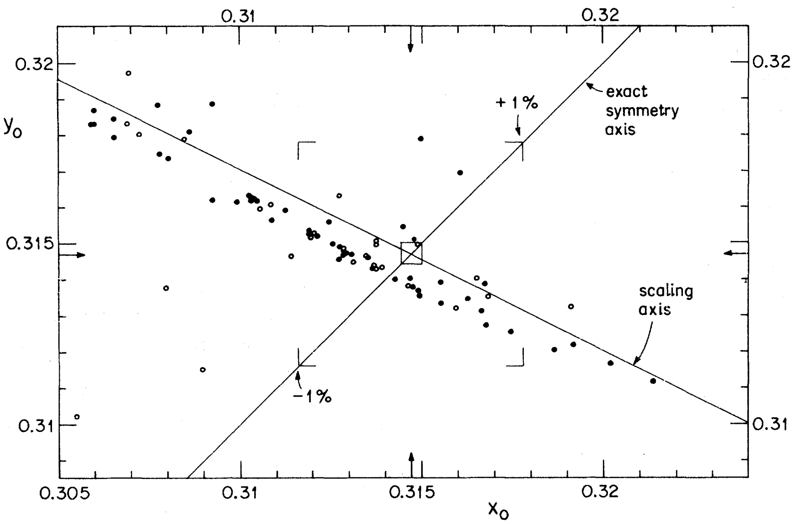

FIG. 1. Scatter diagram in the ($x = J_{\parallel}/k_BT, y = J_{\perp}/k_BT$) plane showing estimates (x_0, y_0) of the location of the multicritical point. Open circles denote lower order PDA's; closed circles, those of higher order. Note the 0.1% and 1% "boxes" about the best estimate, and the scaling axes.

lines enter the multicritical point to form a characteristic *bicritical* cusp,[5b,5c] of shape determined by the crossover exponent ϕ. It is this crucial behavior that is very hard to obtain properly when one is restricted to single-variable analysis.[6]

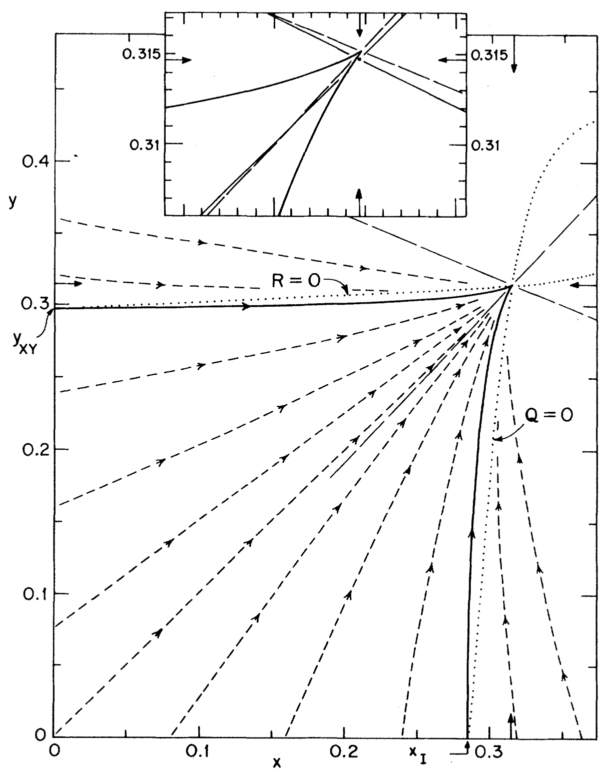

FIG. 2. Trajectories in the (x,y) plane for a [13,12, 12] approximant; see text. The inset shows the (approximate) critical lines in detail in the multicritical region; here the dot and solid lines represent best estimates of the multicritical point and scaling axes.

The unbiased estimates of γ and ϕ corresponding to Fig. 1 are plotted vs x_0 in Fig. 3. (Because of the correlation noted in Fig. 1, this is almost

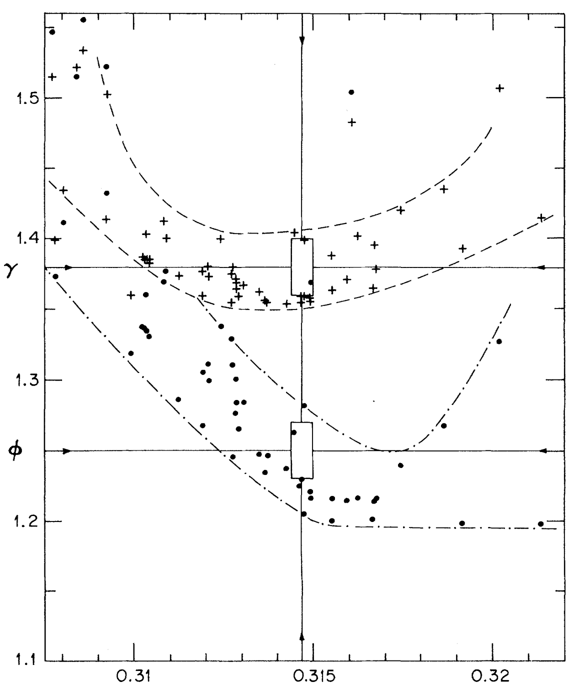

FIG. 3. Unbiased estimates of the multicritical exponents γ and ϕ vs x_0 for approximants with $K \geq 28$. The dashed and dot-dashed curves serve only to indicate the trend of the estimates.

equivalent to a plot vs g.) The "boxes" in the figure denote the range of accepted values. As in ordinary D log Padé analysis,[1-3] a pronounced correlation between exponent and multicritical point estimates is observed. For the central estimates having $x_c \simeq y_c$ ($g \simeq 0$), remarkably good exponent values are achieved. (Again, biased estimation procedures will yield better estimates.) Finally, a similar plot of the estimates for the scaling-axis slopes, e_1 and e_2 (for which there are no analogs in single-variable analysis) once again reveals quite encouraging agreement with the exact results although a much stronger variation with x_0 is observed.

In summary, we have demonstrated that partial differential approximants provide a theoretically powerful and numerically promising approach to the analysis of power series in two variables in cases where the singularity structure plays a dominant role.

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[1]See G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).

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

[3]See also, e.g., M. E. Fisher, Rep. Prog. Phys. 30, 615 (1967), and Rocky Mount. J. Math. 4, 181 (1974).

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[10]Compare with E. K. Riedel and F. J. Wegner, Phys. Rev. B 9, 294 (1974); and D. R. Nelson, Phys. Rev. B 11, 3504 (1975).

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