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Series analysis of tricritical behaviour: mean-field model and partial differential approximants

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Abstract. A partial differential approximant (PDA) analysis of series for the tricritical point of the mean-field model of Glasser, Privman, and Schulman has been developed. All features of the tricritical point are exactly reproduced by an overwhelming majority of the trial PDAs in contrast to the mixed success of the slicewise Padé approximant method. The effect of noise on the approximant convergence is also studied.

1. Introduction

We report here on a substantial advance in the development of algorithms for the numerical investigation of tricritical behaviour in a two-variable phase diagram. Such a method of analysing series for models with a tricritical point has been an elusive aim for many years in the context of both magnetism and polymer studies. A full review of the physical systems exhibiting tricriticality and previous calculations in both a series and a simulation context has recently been given by Adler and Privman [1]. These authors derived a test series based on a mean-field model with a tricritical behaviour which is well understood and has most of the features of 'real' tricritical points of two-dimensional (2D) and three-dimensional (3D) systems. We will summarize the features of the model in section 2.

The only reliable method for studying tricritical points from series expansions that has been applied to date is matching high and low temperature series, when available [2]. Some early studies [3] also used a standard 'slicewise' Padé method. In [1] this method was applied to the 'test' series of the mean-field model. While those features of the Padé approximant approach which can be regarded as signatures of a tricritical point in the phase diagram, and which were noted in early studies of tricriticality [3], were identified, it was concluded, that this most straightforward Padé method is not suitable as an accurate and systematic analysis technique. In the present paper we describe our development of a systematic method, based on elaborations of the two-variable partial differential approximant (PDA) techniques used successfully for bicritical points [4]. The analytic solution with PDAs is given in section 3 and the numerical solution is given in section 4. Section 5 is devoted to concluding remarks.

2. The mean-field model

The models of Glasser *et al* [5], avoid some pathologies common to other infinite-range models. They have a 'soft' temperature (T) dependence which is an artefact of the infinite-range model, and there are some other artificial features near $T = 0$, but the series is well

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defined and can be derived in closed form to any fixed order given sufficiently powerful computational facilities.

The model has interacting scalar spins, σ_i, with energy

$$E = -\frac{J}{2N}\left(\sum_{i=1}^{N}\sigma_i\right)^2 \tag{2.1}$$

where N is the number of spins, and $J > 0$.

The Gaussian-integral method [5] was used to show that in the limit $N \to \infty$ the dimensionless free energy, f, can be obtained as

$$f = \min_x \left[\frac{kTx^2}{2J} - Q(x)\right] \tag{2.2}$$

where

$$Q(x) = \ln \int \mathrm{e}^{x\sigma}\, \mathrm{d}\mu(\sigma). \tag{2.3}$$

The spins are weighed with measure $\mathrm{d}\mu(\sigma)$ in the partition function from whence the free energy is obtained, and the variable x [5] is equal to $y(2J/kTN)^{1/2}$, where y is the variable introduced in the Gaussian integral. If the minimum in (2.2) is at some $x = x_m$, then one can further show that the magnetization, m, is

$$m = \left(\frac{\mathrm{d}Q}{\mathrm{d}x}\right)_{x=x_m} = \frac{kTx_m}{J} \tag{2.4}$$

where the last equality follows from the fact that the global minimum is obtained at one (or more) roots of

$$\frac{\mathrm{d}Q}{\mathrm{d}x} = \frac{kTx}{J}. \tag{2.5}$$

Thus, we note that $m = kTx_m/J$, i.e. $m \propto T$ for low temperatures. This is one of those artificial infinite-range model features. It is convenient to work with x_m directly rather than with m, as the order-parameter-like quantity for series analysis. Of course, the actual critical–tricritical first-order behaviour is at $T > 0$ so the difference only affects the form of analytic corrections to scaling.

In order to have a solvable model with tricritical behaviour, $Q(x)$ was taken as an even, six-degree polynomial in x, the *actual series* was conveniently generated [1] for

$$x_m\sqrt{3} = \sqrt{\sqrt{(U-1)^2 - 3(T-1)} + U - 1} \tag{2.6}$$

where U is a dimensionless coupling constant just as T is a dimensionless temperature in this model. Using *Mathematica*, the order 50 double series in T and U for this order-parameter quantity was derived in [1]. It is expressed as the first 2601 coefficients c_{ij}, for $i, j = 0, \ldots, 50$, in

$$\sqrt{3}x_m = \sum_{i=0}^{50}\sum_{j=0}^{50} c_{ij}T^iU^j. \tag{2.7}$$

An analysis of the exact solution [1] showed that $U_c = T_c = 1$, and that near the tricritical point, one can write the low-T-side scaling form in terms of the scaling variables

$$t = T - 1 < 0 \qquad \text{and} \qquad u = U - 1 \tag{2.8}$$

$$\sqrt{3}x_m \simeq (u)^{1/2} Z_-\left(\frac{-t}{u^2}\right) \tag{2.9}$$

where the scaling form (2.9) applies for $t, u \to 0$ and the scaling function is

$$Z_{-}(\zeta) = \sqrt{1 + \sqrt{1 + 3\zeta}}. \tag{2.10}$$

3. An analytic solution by PDA

The PDA method was developed by Fisher and co-workers [6–8] for two-variable series analysis and extrapolation. It allows us to estimate the critical parameters for functions with the following asymptotic form

$$f(t, u) \approx |u|^{-\gamma} Z\left(\frac{-t}{|u|^{\phi}}\right) + B \tag{3.1}$$

near the critical region, which is satisfied at both bicritical points [6, 7], and tricritical points [9]. For bicritical points, analyses were made by Fisher [6, 10] for the Ising–Heisenberg XY model, and for the 2D Ising model by Styer [8]. The numerical analysis of the Ising–Heisenberg XY model [6, 10] yielded good results for the bicritical point, the critical exponents, and the scaling slopes. For the 2D Ising model, we have an analytic solution for the magnetization [8], and PDAs have an exact solution in this case; the numerical results were very accurate in this case and these will be given in [11]. Just as for the simpler single-variable Padé approximants, our aim is to calculate approximants to $f(t, u)$ and then obtain estimates of the critical parameters from these approximants.

From a comparison between equations (3.1) and (2.9) we can see that for the model defined above that we will study, we expect to obtain the results $\gamma = -0.5$ and $\phi = 2$. The tricritical point in this model [1] is at $U = T = 1$. The generating equation of the PDA [6] is

$$V_J(T, U) + P_L(T, U)F(T, U) = Q_M(T, U)\frac{\partial F(T, U)}{\partial U} + R_N(T, U)\frac{\partial F(T, U)}{\partial T} \tag{3.2}$$

where $F(T, U)$ is the solution of the generating equation, $V_J(T, U)$, $P_L(T, U)$, $Q_M(T, U)$, and $R_N(T, U)$ are polynomials in the two variables U and T. These have non-zero coefficients on the sets J, L, M, and N, respectively, of coefficient values. (It is more usual to use U_J, rather than V_J but since U was used as a variable for our model, we use V for the polynomial.) There is another set, K, which is called the matching set which determines the matching coefficients of f and F, i.e. if the series expansion of the solution $F(T, U) = \sum_{i,j=0}^{\infty} c_{ij} T^i U^j$ and that of $f(T, U) = \sum_{i,j=0}^{\infty} f_{ij} T^i U^j$, then $c_{ij} = f_{ij}$ for all $(i, j) \in K$. In our case

$$f(T, U) = x_m\sqrt{3} = \sqrt{\sqrt{(U-1)^2 - 3(T-1)} + U - 1} \tag{3.3}$$

and we have found that the generating equation (3.2) has an exact analytic solution for $f(T, U)$ in equation (3.3). This is the PDA that will be referred to hereafter as the minimal approximant:

$$\begin{aligned} V(T, U) &= 0 \\ P(T, U) &= 1 \\ Q(T, U) &= 4(T-1) \\ R(T, U) &= 2(U-1). \end{aligned} \tag{3.4}$$

Applying PDAs to a two-variable series of a function with the scaling form (3.1), one finds the multi-critical point (T_c, U_c) (tricritical in our case) to be approximated as the common zero (T_0, U_0) of $Q_M(T, U)$ and $R_N(T, U)$. Solving the generating equation (3.2) near the multi-critical point for the scaling form (3.1) one can see [6] that the critical parameters of (3.1) satisfy the relations:

$$\gamma = -\frac{P_0}{R_2 - e_2 Q_2} \qquad \phi = \frac{Q_1 - R_1/e_1}{R_2 - e_2 Q_2} \qquad B = -\frac{V_0}{P_0} \tag{3.5}$$

where

$$\begin{aligned} &P_0 = P(T_0, U_0) \qquad V_0 = V(T_0, U_0) \\ &Q_1 = \frac{\partial Q(T_0, U_0)}{\partial T} \qquad Q_2 = \frac{\partial Q(T_0, U_0)}{\partial U} \\ &R_1 = \frac{\partial R(T_0, U_0)}{\partial T} \qquad R_2 = \frac{\partial R(T_0, U_0)}{\partial U} \end{aligned} \tag{3.6}$$

and the scaling slopes e_1, e_2 which can be defined from

$$\begin{aligned} &t = (T - T_0) - \frac{(U - U_0)}{e_1} \\ &u = (U - U_0) - e_2(T - T_0) \end{aligned} \tag{3.7}$$

are the solutions of

$$Q_2 e^2 + (Q_1 - R_2)e - R_1 = 0. \tag{3.8}$$

For our model, a comparison of equation (2.8) with equation (3.7) shows that the two roots of equation (3.8) should be $e_1 = -\infty$ and $e_2 = 0$. Using the exact solution (3.4) to substitute the numerical values of (3.6) into (3.5), and substituting the solution of (3.8) into (3.7) one can easily see that for the case we are dealing with indeed we obtain the exact results

$$\begin{aligned} &T_0 = 1 \qquad U_0 = 1 \\ &\gamma = -0.5 \qquad \phi = 2 \\ &e_1 = -\infty \qquad e_2 = 0. \end{aligned} \tag{3.9}$$

These are in agreement with the parameters of the full solution as given above.

4. Numerical analysis

In order to explain our analysis and to provide an exposition of the PDA method we now commence a careful description of the implementation of the PDA solutions. We will discuss both exact sets which include the minimal exact solution of the previous section and solve the generating equation and other approximate sets which also include the minimal exact solution. We begin by describing one set in detail and then repeat the procedure for the other sets without giving all the details. The first non-minimal exact set to be used in solving the PDAs is given in table 1. This set has been selected to be fairly small for ease of explanation but not so small that characteristic features are lost. The table uses the graphical notation developed by Fisher [6] and used by Styer in his published program [7]. In this graphical notation one gives each two-variable polynomial $\sum_{i=0}^{n}\sum_{j=0}^{m} a_{ij} T^i U^j$ a $(n \times m)$ matrix of X's and blanks, an X in the (i, j)th element means that a_{ij} can take values other than 0, while a blank in the (i, j)th element means $a_{ij} = 0$. This graphical notation aids us to visualize the shape of the polynomials in the two-variable space.

Table 1. The sets J, L, M, and N, corresponding to the approximant of equation (4.1).

The set J of coefficients of V	The set L of coefficients of P
	XX
	X
	X
The set M of coefficients of Q	**The set N of coefficients of R**
XXX	XX
XX	XX
XX	X
	X

Table 2. The sets K used with the first approximant, all with $|K| = 16$.

#1	#2	#3	#4	#5
XXXXX	XXXXX	XXXX	XXXXX	XXXX
XXXX	XXXXX	XXXX	XXXXX	XXXX
XXX	XXX	XXXX	XXXX	XXXX
XX X	XX	XXXX	XX	XX
X	X			XX
#6	**#7**	**#8**	**#9**	**#10**
XXX	XXXXX	XXXXXX	XXXXXX	XXXXXX
XXX	XXX	XXX	XXXX	XX
XXX	XXX	XX	XX	XX
XXX	XXX	XX	X	XX
XX	X	X	X	XX
XX	X	X	X	X
	X	X	X	X

The polynomials themselves (which solve the generating equation in our case) are:

$$
\begin{aligned}
V(T,U) &= 0\\
P(T,U) &= p[(U-1)^2 - 3(T-1)]\\
Q(T,U) &= 4p(T-1)[(U-1)^2 - 3(T-1)]\\
R(T,U) &= 2p(U-1)[(U-1)^2 - 3(T-1)]
\end{aligned}
\tag{4.1}
$$

where p is a constant parameter.

As we can see directly from (4.1) V is zero so all rows and columns have blanks in the J set. The expansion of (4.1) is

$$
\begin{aligned}
P_L(T,U) &= p_{00} + p_{10}T + p_{01}U + p_{02}U^2\\
Q_M(T,U) &= q_{00} + q_{10}T + q_{20}T^2 + q_{01}U + q_{11}TU + q_{02}U^2 + q_{12}TU^2\\
R_N(T,U) &= r_{00} + r_{10}T + r_{01}U + r_{11}TU + r_{02}U^2 + r_{03}U^3
\end{aligned}
\tag{4.2}
$$

where p_{ij}, q_{ij}, and r_{ij} are such that in table 1 i denotes columns and j denotes rows. In the present model $p_{00} = 4p$; $p_{10} = -3p$; $p_{01} = -2p$; $p_{02} = p$ etc it is because of

Table 3. The other approximant sets J, L, M, N, and K.

#	J	L	M	N	K	#	J	L	M	N	K
1	XX X	X X X	XXX XX X	XX X X X	XXXXX XXXX XXX XX X X	2	X	XX XX X	XXX XXX XX	XXX XX X X	XXXXXX XXXXXX XXXX XXX X
3	XXX XX X	XX XX XX	XXX XX X	XX XX X	XXXXX XXXXX XXXXX XXXXX XX	4		XXXX X X	XXX XXX XX X	XX XX	XXXXXX XXXXX XXXX XX X
5		X X X	XXX XXX XXX	XXX XX X X	XXXXX XXXXX XXXX XX XX	6	XXXX XXX XX X	XXX XX X	XXXX XXX XX X	XXXX XXX XX X	XXXXXXXX XXXXXXX XXXXXX XXXXX XXXX XXX XX
7	XX X	XX	XXX XX	XX XX X X	XXXXX XXX XXX XXX X	8		XXX XXX XXX	XXX XXX XXX	XX XX XX XX	XXXXXX XXXXX XXXX XXXX XXX XX X
9		XXX XXX X	XXXX XXXX XX	XXX XXX XX X	XXXXXXX XXXXX XXXX XXX XXX XX X	10		XXXX X X	XX XX XX	XXX XX XX X	XXXXXX XXXX XXX XXX XX X

the exact solution that we are able to specify the coefficients. When no exact solution is avaliable a polynomial of the same shape would still be indicated by two X's in the first row corresponding to the non-zero constant term, p_{00}, and T coefficient p_{10}, and those in the first column of the second and third rows, correspond to the coefficients p_{01} and p_{02} for U and U^2, correspondingly. Similarly for the coefficients of Q and R; we can see that the three X's in the first row of the set M correspond to the constant, T and T^2 terms. For this first non-minimal set we checked that it is an analytic solution and that it gives results identical to the minimal exact approximant.

For the numerical analysis we used 15–35 terms of the series, making analyses with many different generalizations of the minimal approximant. Finally, we added 'noise' to mimic series with numerical uncertainties. To solve the generating equation numerically we used a Fortran program, based on Styer's PDA subroutine library [7]. We tested our version of the program by repeating the bicritical analysis of [6, 8, 10], and wish to note that this validation was complicated by problems with the published tables of the bicritical

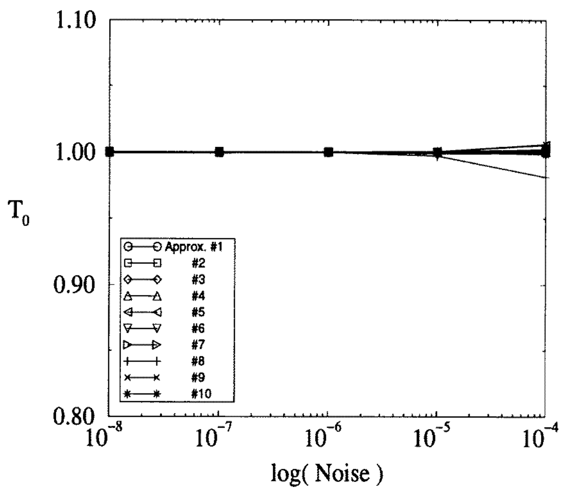

Figure 1. The value of T_c approximated as a function of noise for the first approximants.

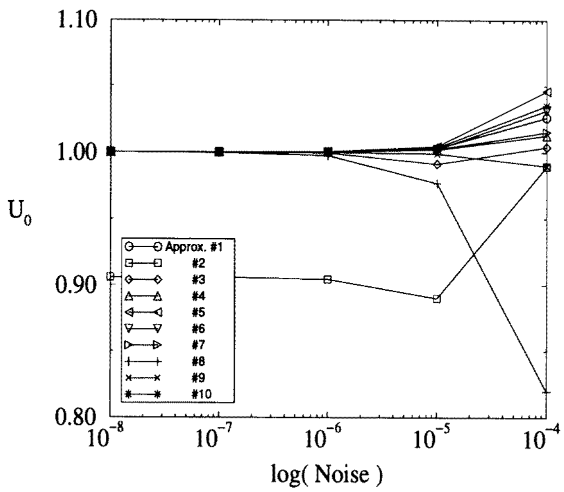

Figure 2. The value of U_c approximated as a function of noise for the first approximants.

series of [12]. Details of this will be given in [11]. Part of our validation was based on material from Styer [8]. We have developed a graphical interface for our version of the PDA routine and would be happy to provide this on request.

Once validation was complete, we first used our program to approximate $f(T, U)$ with the approximant of table 1 and different matching sets K of $|K| = 16$ (see table 2) coefficients from the series (2.7) (to answer the requirement for unconstrained approximants $|K| = |J| + |L| + |M| + |N| - 1$) with the normalization condition $p_{00} = 1$, and then with non-minimal sets (also unconstrained approximants). For example set #1 (from table 2) corresponds to matching the coefficients c_{ij} (with $i = 0, 1, 2, 3, 4$ $j = 0$, $i = 0, 1, 2, 3$ $j = 1$, $i = 0, 1, 2$ $j = 2$, $i = 0, 1, 3$ $j = 3$ and $i = 0$, $j = 4$) of $F(T, U)$ with the corresponding coefficients of $f(t, u)$. All the approximants from tables 1 and 2 gave the exact result of $T_0 = U_0 = 1$, $\gamma = -0.5$, $\phi = 2$, $e_1 = -\infty$, and $e_2 = 0$.

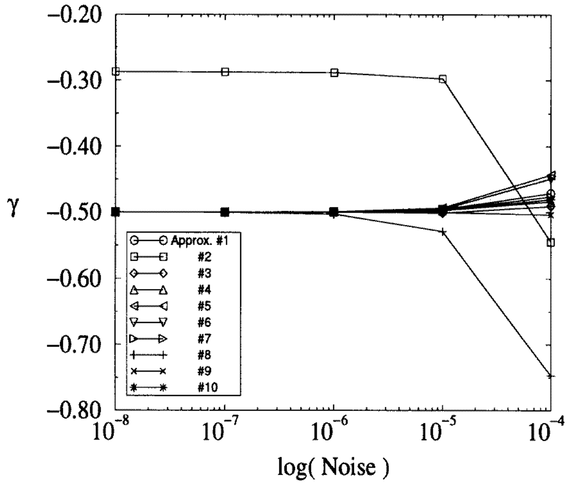

Figure 3. The value of γ approximated as a function of noise for the first approximants.

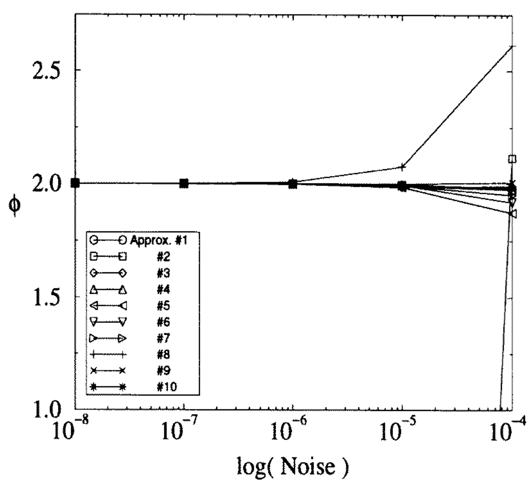

Figure 4. The value of ϕ approximated as a function of noise for the first approximants.

As well as the above described case we solved the generating equation for a second set of other non-minimal approximants (table 3). Similarly to the case of the first approximants all other approximants gave correct results, but one approximant (#1 from table 3) gave the following results: $T_0 = 1.0216$, $U_0 = 1.168$, $\gamma = \phi = 0$, and $e_1 = e_2 = 0$, for which we have no explanation.

To examine the stability of the approximants and to mimic series that are not expansions of exact solutions better we inserted increasing amounts of noise into the series. The noise was introduced by randomly changing the coefficients of the series in the following way: $c_{ij} = c_{ij} + N \times R$; where N is the noise amplitude taking the values 0.0001, 0.000 01, 0.000 001, 0.000 0001, and 0.000 000 01, while R is a random number in the interval $[-1, 1]$.

For the first approximants one can see in figures 1 and 2 that as the noise in the coefficients is reduced, the value of the approximated T_c and U_c converges to 1 as expected, except for approximant #2 which approaches to $T_0 = 0.9993$ and $U_0 = 0.906$.

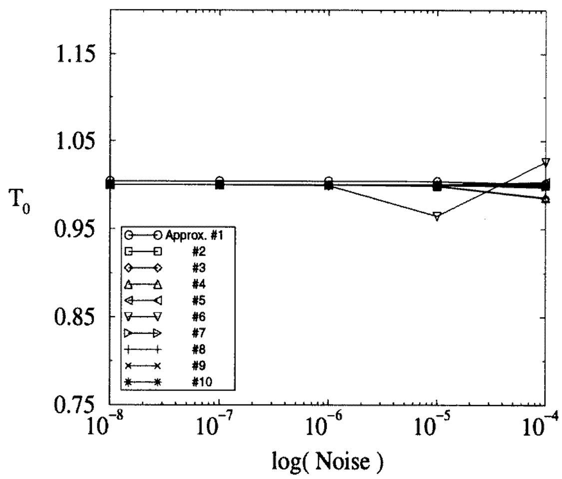

Figure 5. The value of T_c approximated as a function of noise for the second approximants.

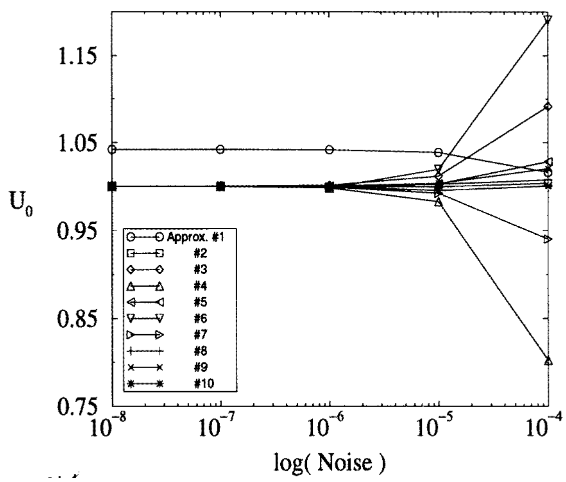

Figure 6. The value of U_c approximated as a function of noise for the second approximants.

Similarly in figures 3 and 4 one can see that the values of the exponents γ and ϕ converge to -0.5 and 2 correspondingly; except for approximant #2 which converges to $\gamma = -0.2875$ and $\phi = -5091$. Notice that approximant #2 gives bad results for both the tricritical point and the critical exponents, though in the case of critical exponents the errors were considerably larger.

For the second approximants the results were also very encouraging as one can see from figures 5 and 6, which show the values of the approximated T_c and U_c, correspondingly, as a function of noise. We can see that except for approximant #1, which converges to $T_0 = 1.004$ and $U_0 = 1.042$, all approximations converge to 1.

Similarly the approximated values of the exponents γ and ϕ converge to -0.5 and 2 correspondingly, as can be seen in figures 7 and 8, except for approximant #1, which converges to $\gamma = -0.4334$ and $\phi = 1.888$. Note that approximant #1 does not yield exact results for either the tricritical point nor the critical exponents, with and without noise. We

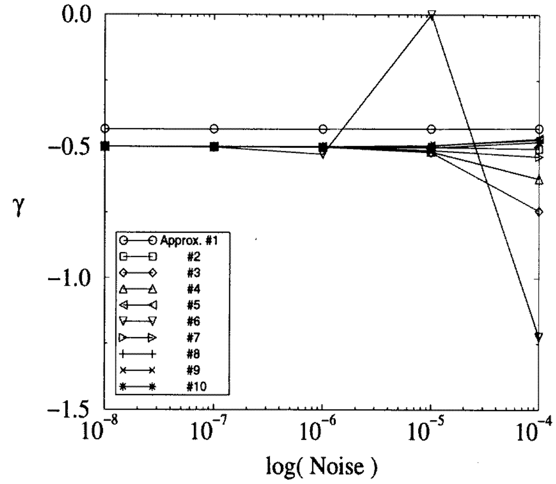

Figure 7. The value of γ approximated as a function of noise for the second approximants.

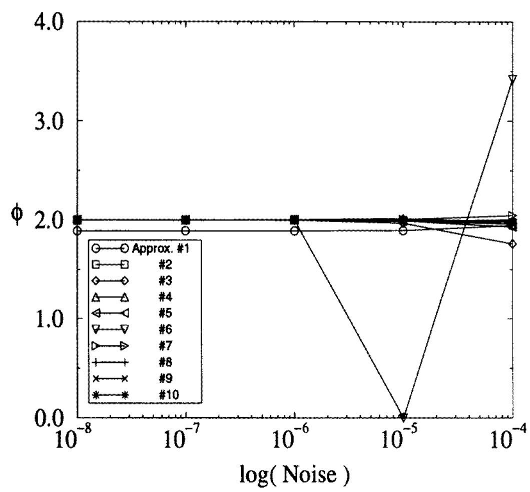

Figure 8. The value of ϕ approximated as a function of noise for the second approximants.

are not certain what causes this deviation; however, it is very clear that in each sample nine of the ten give exact results and so the defective one can be discarded. This is a higher typical success rate than occurs in many Padé-type analyses.

5. Conclusions

We have made an accurate characterization of a tricritical point from a series expansion. The minimal exact approximant, and 18 of the other 20 approximants converged with many significant figures to the exact results. The other two had errors mostly of a few percent. The addition of noise enabled us to explore the nature of the convergence under more realistic conditions. We found pleasing convergence to the exact results, even for noise levels far larger than would be found in series calculated with typical precision. We intend to apply the method to various other series [2, 3] describing tricritical points in the near future.

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