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Series analysis of tricritical behaviour: mean-field model and slicewise Padé approximants

Joan Adler†§ and Vladimir Privman‡

† Department of Physics, Technion—Israel Institute of Technology, Haifa 32000, Israel

‡ Department of Physics, Clarkson University, Potsdam, NY 13699–5820, USA

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Abstract. A mean-field model is proposed as a test case for tricritical series analysis methods. Derivation of the 50th-order series for the magnetization is reported. As the first application this series is analysed by the traditional slicewise Padé approximant method popular in earlier studies of tricriticality.

1. Introduction

Development of algorithms for the numerical investigation of tricritical behaviour in a two-variable phase diagram has been an elusive goal for many years in the context of both magnetism and polymer studies. Two such systems that have been the focus of special interest are random field models for which the tricritical point is expected in the two-parameter space of temperature and randomness strength [1], and the θ -point transition of linear polymers [2] for which the second variable is the ‘stickiness’ fugacity leading to collapse. For these and other systems with tricritical points, all the standard large-scale numerical methods have been utilized: Monte Carlo [3–5] and transfer matrix techniques [5, 6] (the latter for 2D models), and series analysis [7].

There are many complicating factors for such studies. The models involved are rarely simple and must be analysed at multiple points in the two-parameter space. A ‘test problem’ with an exact solution and a series expansion (such as the 2D Ising model which is widely used in calibrating new techniques for second-order transitions) has been missing until now for two-variable problems with tricritical points.

Some of the technical problems are specific to the numerical technique. In the random field and θ -point transition models reaching true equilibrium in Monte Carlo simulations, for instance, is complicated by slowdown effects in the low-temperature or dense (collapsed) regions of the phase diagram. We shall not address simulations further in this paper but note that there is considerable controversy over tricritical behaviour between different recent studies of the 2D collapse transition [4]: θ versus θ' points, etc.

Series expansions do not suffer from equilibration problems, and in many cases lattice models are amenable to the generation of series for all points in the two-variable phase diagram. In particular, two-variable series have been developed for both Ising random field (15th-order in general dimension) [1] and several polymer problems [2]. However, for series the main complication is that the very nature of the tricritical behaviour means that techniques for studying both first- and second-order transitions must be applied. While

§ E-mail: phr76ja@technion.technion.ac.il

excellent techniques for identifying first-order transitions via simulation have recently been developed [8], methods to identify first-order transitions from series expansions are unreliable [9] unless both low- and high-temperature series exist. In one notable case (the FCC-lattice Blume–Capel model) where such expansions on both sides of the transition were developed [10] a satisfactory characterization of tricriticality was made from series.

Despite the absence of a systematic, well tested approach to studying tricriticality when series from only one temperature direction are available, some attempts to do so have been made. The variety of the makeup methods used frequently resulted in differences in answers to the basic question concerning the existence of a tricritical point, not to speak of exponent and other parameter estimates which could be attributed to the diversity of methods rather than to the quality of the series expansions available.

This work reports two developments towards systemizing tricritical series analysis. Firstly, we derive 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 2D and 3D systems. Secondly, we apply the standard ‘slicewise’ Padé method to this new series. We identify 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 some early studies of tricriticality by series [7].

We conclude, however, that this most straightforward Padé method is not suitable as an accurate and systematic general analysis technique, and it can be only used for exploratory studies or in conjunction with other information. Application of the slicewise Padé method to certain random-field model series will be reported in a forthcoming publication. However, the door is still wide open for developing a systematic series-analysis method, possibly based on elaborations of the two-variable differential approximant techniques used successfully for bicritical points [11].

One interesting aspect of our test series derivation, reported in section 2, and its Padé analysis in section 4, is that both rely heavily on novel large-scale computational abilities. Series derivation required a large *Mathematica* run, whereas Padé analysis, employing simultaneously many Padé-pole calculations and extensive graphics representations of the data, revealed new features not accessible to earlier studies from the seventies [7]. Thus, future tricritical series analysis are likely to be large-scale computational projects. Section 3 summarizes the tricritical phase diagram of the mean-field model used in test-series studies. Finally, section 5 is devoted to some concluding remarks and to acknowledgments.

2. The mean-field model

In this section we report derivation of a low-temperature two-variable series for a tricritical point in an infinite-range model with mean-field critical behaviour. There are two kinds of solvable Ising-type infinite-range models. In the first and more familiar type the spins are ± 1 , but their interaction energy, which is the function of the total magnetization, is essentially arbitrary. Usually it is selected (or Taylor-expanded) as a polynomial in the total magnetization so that the resulting constrained free energy, as a function of the magnetization, m , resembles the Landau expansion.

The second type of a mean-field model [12] is defined by having a simple quadratic energy but a complicated entropy-like contribution due to assigning essentially an arbitrary measure in the evaluation of the partition function of a system of scalar spins which vary in $(-\infty, +\infty)$.

Both types of infinite-range models suffer from the difficulty that the low-temperature, T , behaviour is different from the short-range lattice models. Indeed, for short-range models

the low- T series expansions are in terms of the Boltzmann factors of excitations above a reference ground state, of the form $\exp(-\Delta E/kT)$, where $\Delta E = O(1)$ is the energy cost due to a local structure (overturned spins, broken bonds, etc). However, this 'locality' of the excitation structure is lost for infinite-range models. The ± 1 -spin models have entropic contribution to the constrained (fixed- m) free energy with singularities of the type $\sim (1-m)\ln(1-m)$ near magnetization $m = 1$ (and similarly near $m = -1$). Thus setting up a low- T expansion presents a mathematical challenge.

The models of [12] are less troublesome in this respect. One can get a well controlled series in powers of T itself. This 'soft' T -dependence is an artifact of the infinite-range model, and there are some other artificial features near $T = 0$, but the series is well defined and can be derived in closed form to any fixed order given sufficiently powerful computational facilities. Thus, we choose to work with the model of [12] here.

The energy of the interacting scalar spins, σ_i , is taken as

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

where N is the number of spins, and $J > 0$. The partition function is defined as

$$Z = \int \dots \int \exp(-E/kT) \prod_{i=1}^N d\mu(\sigma_i) \quad (2.2)$$

where the spins are weighed with measure $d\mu(\sigma)$. The order parameter is obtained from

$$m = Z^{-1} \int \dots \int \sigma_1 \exp(-E/kT) \prod_{i=1}^N d\mu(\sigma_i) \quad (2.3)$$

The Gaussian-integral method [12] can be used to show that in the limit $N \rightarrow \infty$ the free energy, f , in $Z = \exp(-Nf)$, can be obtained as

$$f = \min_x \left[\frac{kTx^2}{2J} - Q(x) \right] \quad (2.4)$$

where

$$Q(x) = \ln \int e^{x\sigma} d\mu(\sigma) \quad (2.5)$$

If the minimum in (2.4) is at some $x = x_m$, then one can further show that

$$m = \left(\frac{dQ}{dx} \right)_{x=x_m} = \frac{kTx_m}{J} \quad (2.6)$$

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

$$\frac{dQ}{dx} = \frac{kTx}{J} \quad (2.7)$$

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 turns out to be 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, we take $Q(x)$ as an even, six-degree polynomial in x . There is still freedom in selecting the coefficients, etc. We choose to work with dimensionless parameters which, disregarding various dimensional factors, amounts to effectively putting

$$J = k/2 \quad (2.8)$$

$$Q(x) = x^2 + (U - 1)x^4 - x^6 \quad (2.9)$$

so that our choice corresponds to

$$f = \min_x [(T - 1)x^2 - (U - 1)x^4 + x^6]. \quad (2.10)$$

This is the simplest Landau-expanded form to yield the tricritical point, at $(T, U) = (1, 1)$, in the two-parameter space of the (dimensionless) temperature, T , and another (dimensionless) ‘coupling constant’, U .

On the low- T side there are two symmetric roots of (2.7), and there is always one root at $x = 0$. We consider the root $x_m \geq 0$; the *actual series* is conveniently generated for

$$x_m \sqrt{3} = \sqrt{\sqrt{(U - 1)^2 - 3(T - 1)} + U - 1}. \quad (2.11)$$

By utilizing *Mathematica*, we derived the order 50 double series in T and U for this order-parameter quantity. This series, i.e. the first 2601 coefficients c_{ij} , for $i, j = 0, \dots, 50$, in

$$\sqrt{3} x_m = \sum_{i=0} \sum_{j=0} c_{ij} T^i U^j \quad (2.12)$$

can be obtained via electronic mail, from the authors, on request.

We also derived the functions $a_i(U)$ in

$$\sqrt{3} x_m = \sum_{i=0} a_i(U) T^i \quad (2.13)$$

for $i = 0, 1, \dots, 50$. These functions are available in the FORTRAN form, via electronic mail.

3. The tricritical phase diagram

For $U < 1$, there is a second-order transition line at $T = 1$, at which the order parameter approaches zero according to the mean-field law $x_m \propto \sqrt{1 - T}$. The proportionality constant diverges as $1/\sqrt{1 - U}$ for $U \rightarrow 1^-$. At the tricritical point, the order-parameter vanishes according to $\sim (1 - T)^{1/4}$.

For $U > 1$ there is a first-order transition. The line $T = 1$ still have special significance as the mean-field spinodal (see further below) above which the high-temperature, zero-order-parameter phase exists. However, it is not seen in the low- T expansion. The actual

first-order transition line is determined by the condition that the minima at $x_m > 0$ and at $x = 0$ are equal (cf equation (2.10)). A somewhat lengthy calculation yields

$$T = 1 + \frac{1}{4}(U - 1)^2 \quad (3.1)$$

for the first-order transition line at $U > 1$.

Along this line the low- T -side order parameter vanishes according to $\propto \sqrt{U-1}$ as $U \rightarrow 1^+$, i.e. on approach to the tricritical point. However, for fixed $U > 1$, the order parameter is finite at the first-order transition,

$$x_m \sqrt{3} = \sqrt{\frac{3}{2}} \sqrt{U-1} \quad (3.2)$$

from the low- T side, and it vanishes from the high- T side.

In short-range Ising-type lattice models, if one attempts to analytically continue the thermodynamic functions 'through' the first-order line, one encounters an essential singularity at the first-order transition. This singularity is due to droplet excitations; it is weak and its detection in series analysis has rarely been accomplished unambiguously [9]. Specifically, its manifestation within the traditional Padé method aimed at detecting power-law divergences is at best indirect via sequences of weak, alternating poles and zeros of the approximants [9]; see the following sections for further discussion. While the incorporation of this essential singularity must be ultimately a goal for a fully systematic series-analysis method of tricriticality, at the present state of the art and available series lengths, its presence will have little effect in any series study.

There is no essential singularity for infinite-range models as there are no droplet excitations, only uniform ones. When the thermodynamic quantities are continued past the first-order transition, one encounters a spinodal line at which the low- T order parameter $x_m > 0$ ceases to be a local minimum of the constrained free energy. (While at the first-order line it ceases to be the global minimum.) This mean-field spinodal line is at

$$T = 1 + \frac{1}{3}(U - 1)^2. \quad (3.3)$$

The existence of a sharp spinodal-type singularity is an artifact of the infinite-range model. However, for short-range models traces of spinodal-type behaviour have been noted in available-length series analysis [9]. These are artifacts of employing approximants (within Padé or other analysis methods) which fit the data to a form suggestive of a sharp singularity; see [9] for further discussion.

Near the tricritical point, one can write the low- T -side scaling form in terms of the scaling variables

$$t = T - 1 < 0 \quad \text{and} \quad u = U - 1 \quad (3.4)$$

$$\sqrt{3}x_m \simeq (-t)^{1/4} F_-(u(-t)^{-1/2}) \quad (3.5)$$

where the scaling form (3.5) applies for $t, u \rightarrow 0$ and the scaling function is

$$F_-(\zeta) = \sqrt{\zeta + \sqrt{\zeta^2 + 3}}. \quad (3.6)$$

4. Slicewise Padé analysis

The slicewise Padé analysis is perhaps the simplest, single-variable approach to analysing double-series expansions [7]. Thus, we calculate, for fixed U , approximants to the series coefficients a_i in

$$\sqrt{3} x_m(T, U\text{-fixed}) = \sum_{i=0} a_i(U) T^i . \tag{4.1}$$

The coefficients a_i are approximated by

$$a_i \simeq \sum_{j=0}^{j_{max}} c_{ij} U^j \tag{4.2}$$

where in our case $j_{max} = 50$.

The order $[M/L]$ d log-Padé approximant to the derivative $x'_m = \partial x_m / \partial T$ is defined as the rational approximant of the form

$$\frac{x''_m}{x'_m} \simeq \frac{p_0 + p_1 T + p_2 T^2 + \dots + p_M T^M}{1 + q_1 T + q_2 T^2 + \dots + q_L T^L} \tag{4.3}$$

where the derivative x'_m rather than x_m was used in order to have both the numerator and denominator of the left-hand side diverge at their first singularity as T is increased from zero. Specifically, for fixed U , we have

$$x'_m \propto [T(U) - T]^{-B} \tag{4.4}$$

with $T(U) = T_c = 1$, $B = \frac{1}{2}$ at the critical line for $U < 1$, and $T(1) = 1$, $B = \frac{3}{4}$ at the tricritical value $U = 1$. For the infinite-range model $T(U)$ equals the spinodal value (3.3), while $B = \frac{1}{2}$, for fixed $U > 1$. Note that for $U \leq 1$ the exponent B is related to the order-parameter exponent usually denoted by β , via $B = 1 - \beta$.

The coefficients $p_{0,\dots,M}$ and $q_{1,\dots,L}$ are calculated in a standard fashion [13] to have the power series of the right-hand side of (4.3) reproduce the first $M + L + 1$ power-series coefficients of the left-hand side. Of special interest are the poles of the approximant which here depend parametrically on U and will be loosely denoted simply by $T(U)$. It is anticipated that for power-law singularities (4.4) a ‘stable’ pole location will be found in the highest-order, near diagonal approximants (i.e. $M \simeq L$ and $M + L + 1$ close or equal to the order of the available series for x''_m/x'_m) such that for T near $T(U)$ the right-hand side of (4.3) approximates the behaviour suggested by (4.4),

$$\frac{x''_m}{x'_m} \simeq \frac{B}{T(U) - T} . \tag{4.5}$$

Thus, the residue at the stable pole approximates the exponent in (4.4), $-B$.

For essential singularities and other singularities associated with branch cuts, it has been noted [9] that Padé approximants sometimes yield a sequence of alternating weak poles and zeros (zeros of the denominator and numerator, respectively) which mimic the branch cut. However, the Padé method is well suited only for single-variable expansions of functions with power-law singularities. It is worth pointing out that recently exact results were derived for certain models of partially convex lattice vesicles [14] which show tricritical behaviour

with essential singularities at the 'first-order line' of their phase diagram. Double-variable expansions can be derived for these models [15] and possibly used as test series for methods to detect essential singularities, etc. However, we note that the singularities of the models of [14, 15] seem to be natural-boundary-type and differ from droplet-type essential singularities anticipated at Ising first-order transitions.

It is also important to point out that in the slicewise Padé method used here the approximation is two-fold: the coefficients a_i are calculated *approximately* via the truncated series (4.2); the Padé method is applied to the truncated series (4.1). We kept the order of the Padé approximation, $M + L + 1$, at about half the order of the truncation in (4.2), which is $j_{max} = 50$. Still, as examples below illustrate, the method fails for $U \gtrsim 1$ which is presumably due to the truncation (4.2). While the truncation (4.2) is the approach used in the early literature, it is natural to consider improvement of this approximation: we address this issue later in this section.

As our first example, it is useful to consider approximants with only a single pole. For instance, figure 1 shows the pole location for the approximant [19/1]. We note that the approximant becomes 'defective' for $U \gtrsim 1$ in that the location of the pole has nothing to do with the actual spinodal line. Figure 2 also illustrates that the residue provides a poor approximation to the exponent B . The latter, however, can be blamed on our use of the extremely off-diagonal approximant. This 'hooking' of the approximant away from the actual phase-transition line has been noted in earlier studies [7]. The hooking can also be in the direction opposite to that of figure 1, as occurs, for instance, in the [30/1] approximant not shown here.

Study of diagonal and also numerous near-diagonal approximants (only two are actually illustrated here; see figures 3–5) reveals that they indeed significantly improve the exponent

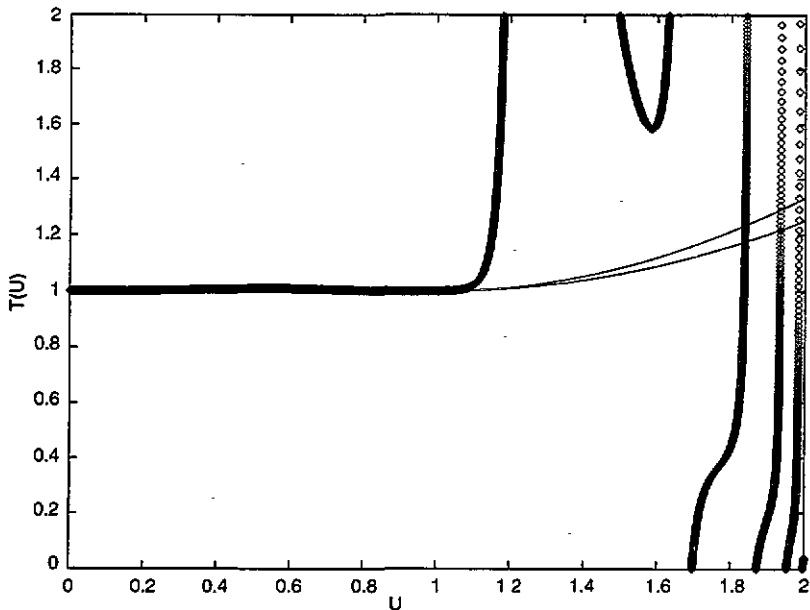


Figure 1. The symbols \diamond , merging for most part as heavy full curves, show the pole $T(U)$ of the [19/1] $d \log$ -Padé approximant to the T -derivative of the magnetization series. The thin full curves correspond to the first-order transition (lower curve, equation (3.1)), and to the mean-field spinodal line (upper curve, equation (3.3)), for $U > 1$. The tricritical point is at $T = 1$, $U = 1$, while for $U < 1$ there is the second-order transition at $T \equiv 1$.

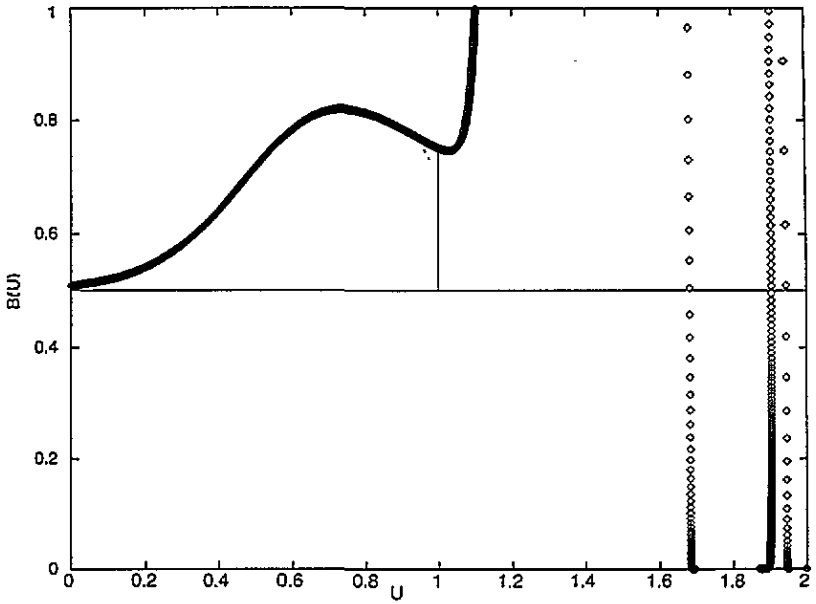


Figure 2. The symbols \diamond show the exponent $B(U)$ as calculated from the residue at the pole of the $[19/1]$ Padé approximant. The horizontal thin full line corresponds to the exact value $B = \frac{1}{2}$ for $U \neq 1$. The vertical spike at $U = 1$ goes up to the exact value $B(1) = \frac{3}{4}$.

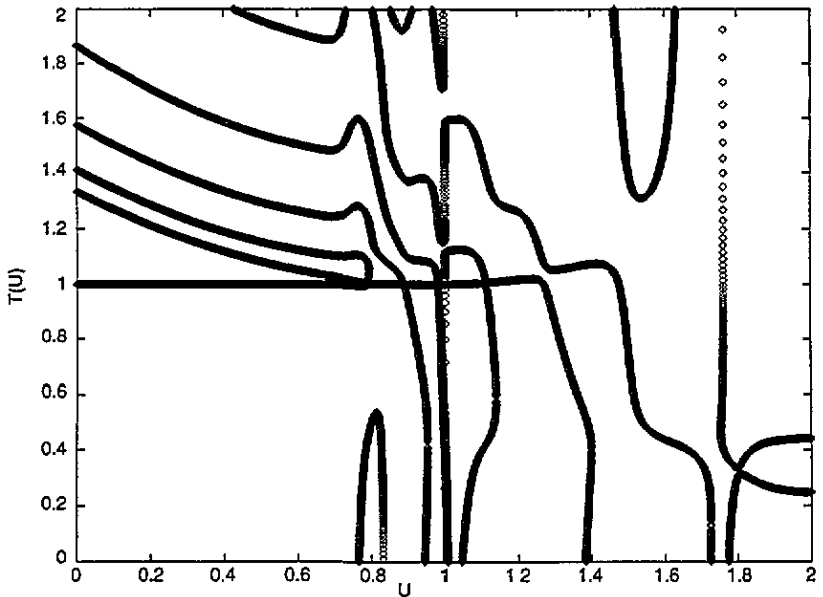


Figure 3. Shown are all the poles $T(U)$ of the $[10/10]$ Padé approximant which fit within the figure range.

B estimate for small $U < 1$. Most approximants also yield B values quite close to $\frac{3}{4}$ at $U = 1$. However, the phase diagram is not well represented near and above the tricritical

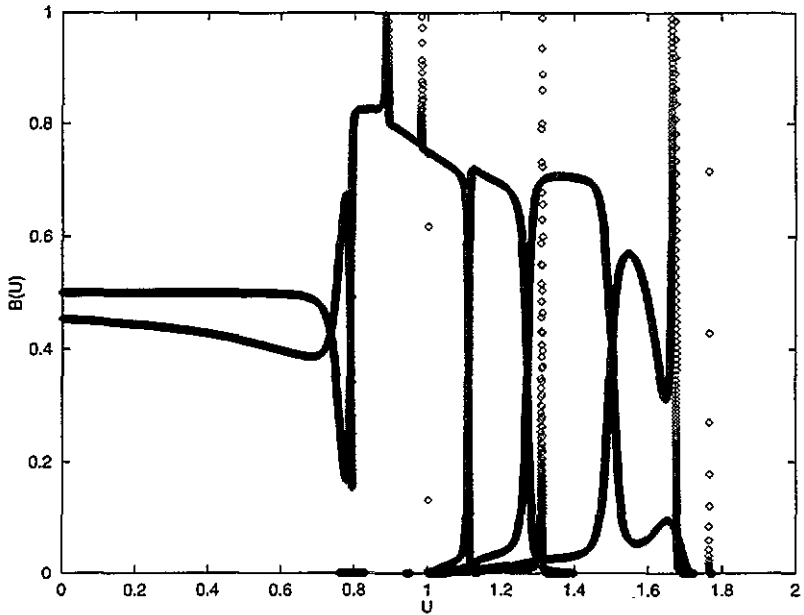


Figure 4. Exponent estimates $B(U)$ from the residues of all the poles of the $[10/10]$ Padé approximant.

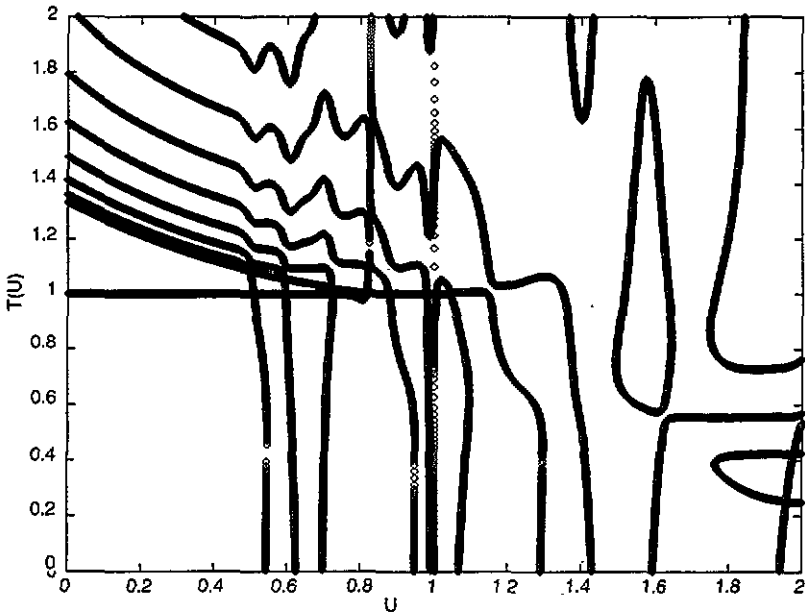


Figure 5. Shown are all the poles $T(U)$ of the $[17/17]$ Padé approximant.

point. In the wide crossover regime near $U = 1$, the approximants become defective: the 'physical' pole alternates among several branches of the roots of the denominator; see figure 3 for the $[10/10]$ approximant. While these branches first roughly follow the exact

spinodal location above $U = 1$, they soon 'hook away'. The exponent estimates also show a rather irregular crossover pattern near $U = 1$; see for instance figure 4 for [10/10]. The approximation fully deteriorates soon above $U = 1$. Furthermore, it seems that the quality of the approximation is affected little by increasing the approximant order as illustrated by the case [17/17] in figure 5.

Our conclusion is that the slicewise Padé method as implemented [7] can at best provide a qualitative indication of the presence of a tricritical point. A wide region of irregular, 'defective' approximant behaviour develops on approach to tricriticality. The hooking noted in earlier studies [7] can be attributed to changeovers among the various pole branches. Thus plotting all the poles and all the residues allows a rough location of the tricritical point and estimation of the exponent. But otherwise the slicewise Padé method should not be regarded as a systematic technique for analysing tricritical behaviour.

We now turn to the approximation involved in the truncation (4.2). Some series actually have the functions $a_i(U)$ as polynomials in U (or other appropriate expansion parameter). However, generally the double-series are available in the form truncated in both variables. It is natural to assume that the quality of the overall can be improved by using resummation methods for the single-variable series (4.2). To our knowledge, no systematic procedures were developed in the literature; one could contemplate Padé or other resummation methods. However, in this work we limited ourselves to the following: we repeated the preceding analysis with the *exact* functions $a_i(U)$, derivation of which was described in section 2.

Figure 6 illustrates the behaviour of the poles for the case of the [10/10] Padé approximant. It should be compared with figure 3. We note that without the truncation (4.2), the approximation for $U \gtrsim 1$ improves. Specifically, the leading pole now clearly follows the spinodal line for $U > 1$. However, the main problems remain: the crossover

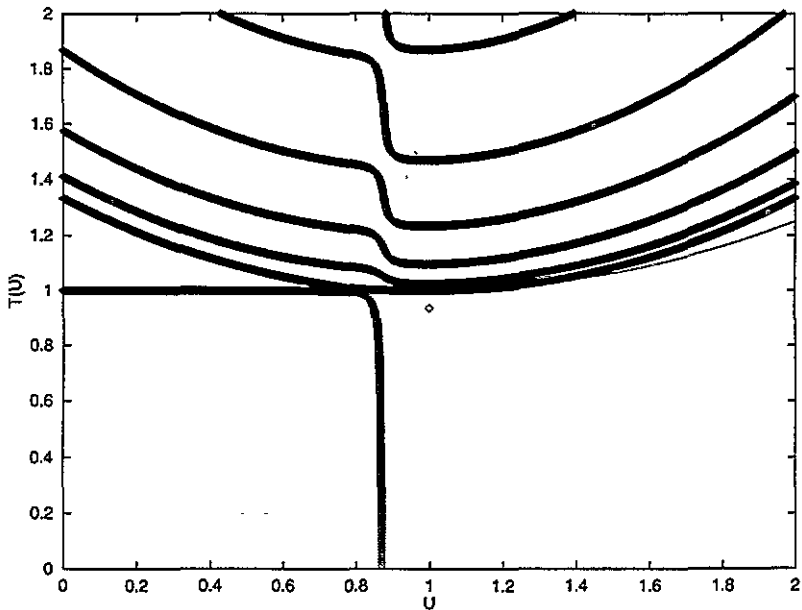


Figure 6. Shown are the poles $T(U)$ of the [10/10] d log-Padé approximant calculated with the exact coefficient values $a_i(U)$ (cf figure 3). For $U > 1$, the thin full line corresponds to the first-order transition (equation (3.1)), while the leading approximant (the smallest $T(U)$ values) follows the mean-field spinodal (equation (3.3)), with the difference smaller than the size of the symbols.

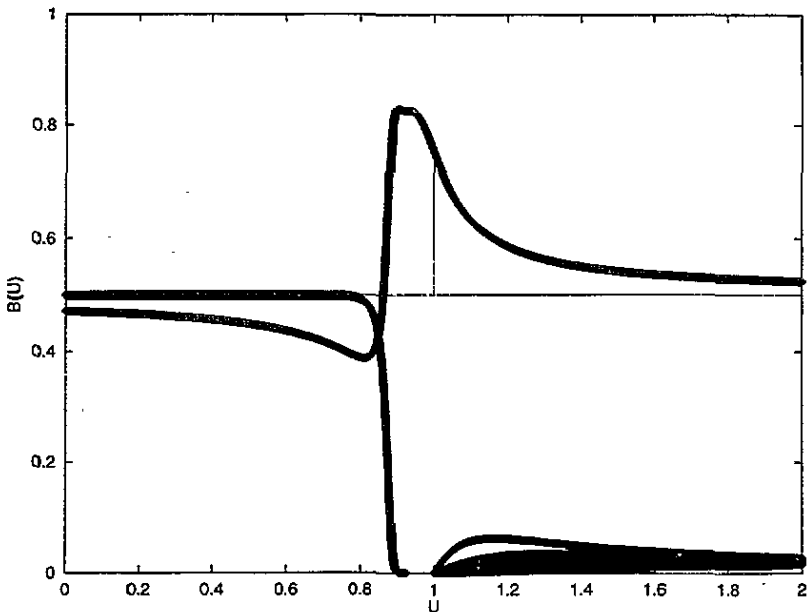


Figure 7. The exponent $B(U)$ as calculated from the residue at the pole of the $[10/10]$ Padé approximant with the exact $a_i(U)$ values; cf figure 4. The horizontal thin full line corresponds to the exact value $B = \frac{1}{2}$ for $U \neq 1$. The vertical spike at $U = 1$ goes up to the exact value $B(1) = \frac{3}{4}$.

region near $U = 1$ is marked by the 'defective' behaviour where poles approach each other and switch role. Furthermore, the leading pole for $U > 1$ is accompanied by a sequence of weak poles which mimic branch-cut effect. Figure 7 shows the residues at the poles of the $[10/10]$ Padé approximant. It should be compared with figure 4. The exponent estimation is only accurate for $U < 1$. In the wide crossover region near $U = 1$ the defective behaviour spoils the accuracy of the approximation, while for $U > 1$ the quality of the approximation is low presumably due to the accompanying weak poles. A similar behaviour was observed for other near-diagonal Padé approximants calculated with the exact $a_i(U)$ values, and as before there was no visible improvement when the order, $[M/L]$, of the approximant was increased.

5. Concluding remarks

As discussed in the previous section, the simplest Padé approach fails in several aspects near tricritical points. Let us now consider a 'wish list' for a more systematic series analysis method. Firstly, we would expect to produce a smoothed-out but regular approximation to the exponent, i.e. the spiked line in figure 2, and to the phase diagram, i.e. to the phase-transition lines shown in figure 1. The approximants should be sharpening up with the increased order of approximation. Secondly, we would also like to estimate the scaling form at the tricritical point, cf (3.5), as in the differential-approximant analysis of bicritical points [11].

An added complication at tricritical points is the presence of singularities at the first-order transition line, as well as possible pseudo-singular spinodal behaviour. Specifically,

for Ising-type models there are weak essential singularities. However, for other models with soft-mode excitations, power-law spin-wave-type singularities are present at the first-order transition. For yet another class of models, the droplet picture may not be fully understood, such as for certain systems with randomness, or the first-order-regime singularities may not have been carefully discussed in the literature, such as for the polymer collapse.

We note that the deterioration of the approximant quality in the slicewise Padé method has always occurred at larger U values. Improvement accomplished by avoiding the approximate truncation (4.2) was not sufficient for really accurate results. Other approaches involve, for instance, 'slicing' along curvilinear paths that originate at the origin of the (T, U) plane, etc. These possibilities will be explored in future publications.

All the above remarks indicate that series analysis of tricritical behaviour promises to become an interesting and active field with the availability of new, long series and modern computational facilities. It is hoped that the approach presented here will yield useful test series for these studies.

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