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1 | Asymptotic Analysis of Power-Series Expansions

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1 Introduction

1.1 Background and scope

There have been a number of significant developments over the past 15 years since the original article on analysis of series coefficients by D. S. Gaunt and A. J. Guttmann was written for this series. At that time, the renormalization group (RG) theory (see Volume 6 of this series) and all its ramifications had yet to become widely known. It was tacitly assumed that most thermodynamic functions had a singularity structure qualitatively similar to that of the two-dimensional Ising model, and most methods of series analysis were variants of the ratio method or the method of Padé approximants. These methods were either applied directly or after an appropriate transformation.

In the intervening years the RG theory produced increasingly precise predictions, some of which were at variance with the beliefs of the time, most notably the series-analysis predictions of the exponents of the three-dimensional Ising model. Reconciliation of many of these differences has occurred, following the explicit inclusion of confluent singularities into methods of series analysis, and many new techniques have been developed to take such singularities into account. While credit for an idea can seldom be assigned to an individual or group, the Illinois group under Michael Wortis appears to have been the first to systematically study confluent singularities in an attempt to reconcile series data with universality for the spin-*s* Ising model.

That work was first reported by Wortis (1970), and a fuller picture of the history and details of earlier contributions is given by Saul *et al.* (1975). Shortly thereafter, Wegner (1972) showed how correction-to-scaling exponents arose naturally within the context of the RG theory, with the first experimental evidence of such terms being reported by Greywall and Ahlers (1972) at about the same time.

The renormalization group also triggered an interest in higher-dimensional systems. The prediction of confluent logarithmic terms at the upper critical dimension provoked an interest in methods of analysis that sought evidence of this term. Quite successful methods were developed by Domb (1974) and Guttmann (1978a).

Another important development was the method of differential approximants. This method was developed by Guttmann and Joyce in 1971 (see Guttmann and Joyce, 1972), following a suggestion of Sykes that the series expansion of the Onsager solution of the two-dimensional Ising model free energy should have coefficients that are related by simple recurrence relations. Joyce found these recurrence relations, and Guttmann developed a method of series analysis based thereon—hence the name "recurrence-relation method". A similar idea occurred to Gammel (1973a) at about the same time. In the method as originally formulated, the underlying function is represented as the solution of a homogeneous differential equation of degree two or higher, with polynomial coefficients. As we discuss in Section 6, this is a "natural" generalization of Padé approximants, and allows in principle for the presence of confluent singularities. Hunter and Baker (1979) subsequently developed the theory appropriate to an inhomogeneous first-order differential equation, and used the more descriptive name of "integral approximants" for the method. Fisher and co-workers in a series of papers considered both the general inhomogeneous case, and perhaps more significantly introduced the idea of "partial differential approximants", which enable series expansions in more than one variable to be studied (see e.g. Fisher, 1977; Fisher and Au-Yang, 1979). We refer to these methods as "differential-approximant" methods, and discuss them in Sections 6 and 7. We consider these methods the most powerful general-purpose class available, and advocate their use as the method of choice in the absence of compelling alternative reasons. This is not to argue that they are always "the best" methods—as we shall see, there is no such thing—but for most of the common singularity structures encountered in models of phrase transitions they represent an excellent starting point.

The work of Kosterlitz and Thouless (1973) on $O(2)$ models in two dimensions predicted a singularity of an entirely different type from the usual algebraic singularity. An essential singularity of the form $\exp[c(x-x_c)^{-\nu}]$ was proposed, and methods of analysis designed to investigate such series were devised by Camp and Van Dyke (1975a), Guttmann (1977), Ferer and Velgakis (1983a) and recently by Butera *et al.* (1989). These and other methods tailored for particular functional

forms—such as Domb's (1976) proposed form for the asymptotic number of lattice animals—will also be reviewed. Section 2 concludes with a discussion of the asymptotic form appropriate to a given singularity structure, and so allows for special methods to be devised, which appropriately generalize the ratio method.

The traditional methods discussed in the earlier article have not been neglected in the intervening years. The theory underlying Padé approximants has advanced significantly, particularly our understanding of the convergence properties of entries in a Padé table. Almost all of this work, and earlier work besides, can be found in the encyclopaedic works of Baker and Graves-Morris (1981a,b) and is summarized in Section 4. A variant of the Padé method due to Nuttall and co-workers (see Baumel *et al.*, 1982a) also shows considerable promise, and is discussed in Section 5. In Section 5 we also discuss the generalized inverse vector-valued Padé approximants introduced by Graves-Morris (1988) and co-workers.

Methods that work directly with the assumed asymptotic form of the series coefficients, such as the ratio method, we call "direct" methods. Padé- and differential-approximant methods are not in this class. New direct methods for conventional singularities have been developed by Zinn-Justin (1979, 1981) and for confluent singularities by Saul *et al.* (1975). There is also a considerable body of numerical-analysis literature for extrapolating sequences, which can be applied to the sequences of ratios and exponent estimates. We review the most successful of these in Section 3.

Another development of significance is the application of methods of series analysis to areas of science other than lattice statistics. M. Van Dyke and co-workers have tackled many problems in the area of fluid mechanics by these techniques, and much of this work is reviewed in Van Dyke (1984). Applications to quantum mechanics and quantum field theory are reviewed in Baker and Graves-Morris (1981b), while applications to simulation and control are described in Graves-Morris (1973).

Several heroic extensions of certain series expansions have also been made, allowing more subtle effects to be probed, and highlighting the danger of excessive reliance on the predictions of series that are insufficiently long for true asymptotic behaviour to manifest iself. The most notable examples are the 21-term b.c.c.-lattice (Nickel, 1982) and 54-term square-lattice high-temperature Ising-susceptibility series generated by Nickel (1985, personal communication), and the 56-term square-lattice and 82-term honeycomb-lattice polygon series generated by Guttmann and Enting (1988a) and Enting and Guttmann (1989). Many other series have been usefully extended by Sykes, Gaunt, Martin, S. McKenzie, Essam and co-workers at King's College and Royal Holloway College and by Butera, Guttmann, D. Hunter, Lüscher, Rehr, Redner, Stanley and Weisz at other universities, to name but a few. The use of these longer series allows the strengths and weaknesses of many analysis techniques to be highlighted.

In this article we propose to assume most of the material in the earlier work of Gaunt and Guttmann, and concentrate on describing the newer methods, or new variants of older methods, that have demonstrated their usefulness over the intervening decade. In order that this article be self-contained, we cursorily review the previous work too. However, we have largely restricted attention to power series with a non-zero radius of convergence; series arising in statistical mechanics are usually (but not always) of this form. Very different techniques are required for power series with a zero radius of convergence. We return briefly to that problem in Section 9.2.

Section 10 constitutes a summary and outlook, and tries to emphasize the philosophy of choosing a method of series analysis that can reflect the expected singularity structure. A cautionary note is sounded about the introduction of untested new methods.

In Section 11 a listing of computer programs for a number of the more widely discussed algorithms is given, along with instructions for their use.

1.2 Basic problem

The simplest and most common problem in series analysis is to determine the parameters A, z_c and λ through

$$F(z) \sim A\left(1 - \frac{z}{z_c}\right)^{\lambda} \quad (z \to z_c). \tag{1.1}$$

where F is some thermodynamic function of the system of interest whose Taylor expansion about the origin is known through the first N terms. That is,

$$F(z) = \sum_{n=0}^{N} a_n z^n, \tag{1.2}$$

where $\{a_n \mid n = 0, 1, \ldots, N\}$ is known. The constants A, z_c and λ are called the critical amplitude, critical point and critical exponent respectively. We frequently drop the adjective "critical".

The case $\lambda = 0$ has several possible interpretations. It could mean that $F(z_c)$ is finite and non-zero, or that $F(z)$ diverges or vanishes logarithmically as $z \to z_c$, for example like

$$F(z) \sim \left|\ln\left(1 - \frac{z}{z_c}\right)\right|^{\alpha} \quad (z \to z_c), \tag{1.3}$$

or in a more complicated form such as $\ln|\ln(1 - z/z_c)|$. If λ is a positive or negative integer, this could indicate a pole or zero of F, or a pole or zero multiplied by a confluent logarithmic term such as (1.3).

The asymptotic form (1.1) is of course only the leading-order term, and it is increasingly clear that in many cases the correction terms need to be taken into account in order to estimate the critical parameters A, z_c and λ with the required degree of accuracy.

The usual form of correction assumed is one or more "correction-to-scaling" terms, characterized by exponents $0 < \Delta_1 < \Delta_2 < \Delta_3 < \ldots$ as in

$$F(z) \sim A\left(1 - \frac{z}{z_c}\right)^{\lambda}\left[1 + A_1\left(1 - \frac{z}{z_c}\right)^{\Delta_1} + A_2\left(1 - \frac{z}{z_c}\right)^{\Delta_2} + \ldots\right] \quad (z \to z_c). \tag{1.4}$$

Note that if $\Delta_i = \lambda$ then this corresponds to a term $A \cdot A_i$ in F. This then is an *additive, analytic term*, and many methods of series analysis cannot distinguish between an additive term of this type and a "genuine" confluent term corresponding to an independent branch of F.

If the exponents Δ_i are all positive integers then $F(z)$ in (1.4) is just the expansion of $F(z) = A(z)(1 - z/z_c)^{\lambda}$, where $A(z)$ is analytic in the neighbourhood of $z = z_c$. If one or more Δ_i are non-integral, we then have one or more confluent singularities.

Confluent terms can also be logarithmic, in which case

$$F(z) \sim A\left(1 - \frac{z}{z_c}\right)^{\lambda}\left|\ln\left(1 - \frac{z}{z_c}\right)\right|^{\alpha} \quad (z \to z_c), \tag{1.5}$$

and special methods are needed to unravel such singularities. Such confluences frequently arise *at* the critical dimensionality of thermodynamic systems, for example the Ising model in four dimensions.

As well as multiplicative confluent singularities, as in (1.5), we can also have additive confluent singularities, in which case

$$F(z) \sim A\left(1 - \frac{z}{z_c}\right)^{\lambda}\left[1 + A_1\left|\ln\left(1 - \frac{z}{z_c}\right)\right|^{-\Delta_1} + \ldots\right]; \tag{1.6}$$

these are also known to occur in model systems (Brézin *et al.*, 1976).

Certain models of interest display quite different singular behaviour from that discussed above. For example, the two-dimensional classical plane-rotator is believed to have a divergent susceptibility of the form

$$F(z) \sim A \exp\left[c\left(1 - \frac{z}{z_c}\right)^{-\sigma}\right] \tag{1.7}$$

(Kosterlitz and Thouless, 1973), as is the one-dimensional Ising model with a ferromagnetic interaction (Anderson and Yuval, 1971). The square lattice *spiral* self-avoiding walk model (Privman, 1983a; Guttmann and Wormald, 1984) has coefficients that diverge like

$$a_n \sim A n^{\gamma} \exp(\delta n^{1/2}). \tag{1.8}$$

For these models, and other special cases, methods of analysis have to be designed to accommodate the assumed functional form.

The last remark highlights the underlying philosophy of all methods of series analysis. This philosophy is that we are fitting series coefficients to an assumed functional form—an assumed form may be implicit or explicit, but is invariably present. This observation is a partial refutation of the purists' objection that the first N terms of a power series will, in principle, tell you nothing of the asymptotic behaviour of the underlying function at points away from the origin. As a mathematical statement, that is incontestable. However, if we assume a certain functional form, including explicit restrictions on subdominant terms, we can say a great deal. The assumed functional forms are motivated by the growing number of exact solutions (Baxter, 1982) and by renormalization-group theory (Brézin *et al.*, 1976).

Nevertheless, it is difficult to quantify errors in any rigorous manner. As a consequence, error bounds are generally referred to as (subjective) confidence limits, and as such frequently measure the enthusiasm of the author rather than the quality of the data. What is clearly required is a comprehensive mathematical treatment of standard methods of series analysis. Such a treatment does not at present exist, though the books by Brezinski (1977), Delahaye (1988) and Wimp (1981) do provide a number of useful results in this direction, within the restricted domain of sequence extrapolation.

1.3 Basic properties of power series

In this section we summarize the properties of power series that lie at the heart of several methods of series analysis, most notably the ratio

method and its variants. Most of this material can be found in standard texts on complex analysis (e.g. Hille 1976, 1977; and Whittaker and Watson, 1963).

Let F be given by

$$F(z) = \sum_{n=0}^{\infty} a_n z^n \tag{1.9}$$

and define

$$\liminf_{n\to\infty} |a_n|^{-1/n} = R. \tag{1.10}$$

Then the series (1.9) converges for $|z| < R$ and defines an analytic function in the disc $|z| < R$; it diverges for $|z| > R$; and if $R < \infty$ (as we assume henceforth), the function F has at least one singular point on the circle $|z| = R$. If $F(z) \sim A(1 - z/z_c)^{-\lambda}$, and the singularity at z_c is the dominant (and hence closest) singularity, then $R = |z_c|$, and the sequence $\{|a_n|^{-1/n}\}$ will give a convergent sequence of estimates of $|z_c|$. Unfortunately, this sequence is rather slowly convergent. For example, let us consider the high-temperature susceptibility series of the square-lattice Ising model, for which 54 terms are known (Nickel, 1985 personal communication):

$$\begin{aligned}\frac{kT\chi_0}{m^2} = {} & 1 + 4v + 12v^2 + 36v^3 + 100v^4 + 276v^5 + 740v^6 + 1972v^7 + 5172v_8 \\ & + 13\,492v^9 + 34\,876v^{10} + 89\,764v^{11} + 229\,628v^{12} + 585\,508v^{13} \\ & + 1\,486\,308v^{14} + 3\,763\,460v^{15} + 9\,497\,380v^{16} + 23\,918\,708v^{17} \\ & + 60\,080\,156v^{18} + 150\,660\,388v^{19} + 377\,009\,364v^{20} + 942\,106\,116v^{21} \\ & + 2\,350\,157\,268v^{22} + 5\,855\,734\,740v^{23} + 14\,569\,318\,492v^{24} \\ & + 36\,212\,402\,548v^{25} + 89\,896\,870\,204v^{26} + 222\,972\,071\,236v^{27} \\ & + 552\,460\,084\,428v^{28} + 1\,367\,784\,095\,156v^{29} + 3\,383\,289\,570\,292v^{30} \\ & + 8\,363\,078\,796\,612v^{31} + 20\,656\,054\,608\,404v^{32} + 50\,987\,841\,944\,612v^{33} \\ & + 125\,771\,030\,685\,740v^{34} + 310\,070\,329\,656\,964v^{35} \\ & + 763\,956\,047\,852\,548v^{36} + 1\,881\,332\,450\,300\,692v^{37} \\ & + 4\,630\,413\,888\,204\,372v^{38} + 11\,391\,558\,864\,854\,532v^{39} \\ & + 28\,010\,951\,274\,197\,380v^{40} + 68\,849\,212\,197\,171\,604v^{41} \\ & + 169\,150\,097\,365\,333\,708v^{42} + 415\,419\,639\,494\,357\,940v^{43} \\ & + 1\,019\,816\,266\,252\,636\,316v^{44} + 2\,502\,715\,799\,503\,410\,388v^{45} \\ & + 6\,139\,555\,263\,040\,186\,116v^{46} + 15\,056\,658\,258\,453\,004\,340v^{47} \\ & + 36\,912\,183\,772\,984\,767\,964v^{48} + 90\,466\,431\,959\,611\,703\,308v^{49} \\ & + 221\,649\,470\,925\,554\,607\,500v^{50} + 542\,914\,755\,497\,182\,676\,020v^{51} \\ & + 1\,329\,440\,077\,424\,712\,435\,476v^{52} + 3\,254\,615\,979\,848\,876\,064\,244v^{53} \\ & + 7\,965\,488\,065\,940\,462\,105\,380v^{54} + \ldots,\end{aligned} \tag{1.11}$$

where $v = \tanh(J/kT)$ is the usual high-temperature expansion variable. The last four terms in the sequence $\{a_n^{1/n}; n = 51, 52, 53, 54\}$ are 2.5501, 2.5481, 2.5462, 2.5444, while the limit of this sequence is known to be $2^{1/2} + 1 = 2.4142135\ldots$, so that the last estimate is still some 5.4% higher than the limit.

A more generally useful theorem (Hille, 1976) is that if

$$a = \liminf_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right| \quad \text{and} \quad A = \limsup_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right|.$$

(so that $a \leq A$) then the series converges for $|z| < A^{-1}$ and diverges for $|z| > a^{-1}$. In most applications $\lim_{n\to\infty}|a_{n+1}/a_n| = |z_c|^{-1}$ exists and is equal to either a or A, and the theorem tells us that the circle $|z| = a^{-1} = A^{-1}$ contains at least one point of non-analyticity. It is worth emphasizing that there may be more than one singularity on the circle $|z| = a^{-1} = A^{-1}$. The high-temperature susceptibility of the spin-$\frac{1}{2}$ Ising model on a loosely packed lattice is an example of such a situation.

If the coefficients of the power series $f(z) = \sum_n a_n z^n$ are all positive for n sufficiently large, Pringsheim's theorem tells us that $z = R$ is a singular point of $f(z)$. Several powerful generalizations of this result exist. For example, the theorem holds under the much weaker condition that $\mathrm{Re}\,(a_n) \geq 0$ for sufficiently large n (Hille, 1976). A corollary of this result, pointed out by A. Sokal, is that if there exists ψ such that $\mathrm{Re}\,(e^{i\psi - in\theta} a_n) \geq 0$ then $f(z)$ has a singularity at $z = Re^{i\theta}$.

The sequence $\{a_{n+1}/a_n\}$ usually converges more rapidly than the sequence $\{a_n^{1/n}\}$. For example, from the series (1.11), the last four ratios are 2.44943, 2.44871, 2.44811, 2.44744, so that the last ratio is some 1.4% away from the limiting value of $2^{1/2} + 1$. In addition to this more rapid convergence, the sequence can be more readily extrapolated than can the sequence $\{a_n^{1/n}\}$, and indeed this observation leads to the ratio method of series analysis, which we consider in Section 2.

A significant amount of information can often be obtained simply by observing the sign pattern of the series coefficients. If they are all positive, or positive after the first k terms, then the closest singularity to the origin lies on the positive real axis. If they alternate in sign, the dominant singularity lies on the negative real axis. If they display a four-term periodicity of sign pattern, there is a conjugate pair of singularities on the imaginary axis. This is in addition to any singularities on the real axis. More complicated singularity locations, such as conjugate pairs of singularities in the complex plane, lead to more complicated, and generally aperiodic, sign patterns.

This behaviour can be clearly understood using Darboux's theorems (1878), which are also useful in our study of correction terms to leading asymptotic behaviour.

1.4 Darboux's first theorem

Suppose that a function F is analytic in the closed disc $|z| \leq \alpha$, †apart from a single algebraic singularity at $z = \alpha$, so that

$$F(z) = (z - \alpha)^{\gamma}\phi(z) + \psi(z) = \sum_n a_n z^n, \tag{1.12}$$

where ϕ and ψ are two functions analytic in the neighbourhood of the closed disc $|z| \leq \alpha$, that is, in some disc $|z| < \alpha + \varepsilon$, where $\varepsilon > 0$. Then the asymptotic form of the coefficients a_n can be obtained by substituting for the expansion of $F(z)$, $(z - \alpha)^{\gamma}$ times the expansion of $\phi(z)$ around $z = \alpha$. Higher order approximations may be obtained by replacing $F(z)$ by

$$\left[\sum_{r=0}^{p} \frac{(z-\alpha)^r \phi^{(r)}(\alpha)}{r!}\right](z-\alpha)^{\gamma}. \tag{1.13}$$

The error in stopping at the pth term is always $O(n^{-(p+1)})$. The proof of this theorem was given by Darboux (1878) and, in a more accessible article, by Szegö (1959). If $p = m$ in (1.13), we refer to this as the $(m-1)$th Darboux approximation.

If $\psi(z) = 0$, this theorem is essentially Taylor's theorem, which states that $F(z)$ may be expanded around the point $z = \alpha$ by taking $(z-\alpha)^{\gamma}$ times the Taylor-series expansion of ϕ around the point $z = \alpha$. The importance of Darboux's theorem is that it tells us that the effect of the additive function $\psi(z)$ becomes vanishingly small. This is intuitively obvious, since it simply states that the asymptotic form of the coefficients of the series expansion of a function is eventually dominated by the closest singularity to the origin. The word "eventually" is the key word here, since the series may be initially dominated by contributions from

† This means that the function is analytic in some *open neighbourhood* of the closed disc.

other singularities. To illustrate this, consider the series expansion of the function

$$f(x) = (1-x)^{-1/4}(1+\tfrac{1}{2}x)^{-3} = 1 - 1.25x + 1.2813x^2 - 0.99219x^3$$
$$+ 0.77881x^4 - 0.50330x^5 + 0.36568x^6 - 0.20517x^7 + 0.15370x^8$$
$$- 0.06987x^9 + 0.06375x^{10} - 0.017169x^{11} + 0.001229x^{12}$$
$$+ 0.016318x^{13} + 0.0069211x^{14} + \ldots \qquad (1.14)$$

If we knew only the first 12 terms of the series, we might guess that the closest singularity to the origin lay on the negative real axis, because the coefficients alternate in sign. It is only after 12 terms that the coefficients "settle down", become of positive sign, and thus indicate that the closest singularity to the origin lies on the positive real axis. Even for this simple function, then, it is possible to deduce quite misleading information if only the first 12 terms of the series expansion are known. It is a trivial exercise to construct much more pathological examples.

The above example gives some insight into the fundamental question of series analysis: "When has the series settled down to asymptotic behaviour?" To answer this question fully is of course impossible, but for the two-dimensional Ising model the exact results provide an excellent testing ground. Consider the spontaneous magnetization of the Ising model on a square lattice, first obtained by Onsager in 1947, though never published by him, for which Yang (1952) obtained the exact result

$$M_0(z) = \sum_{n=0}^{\infty} a_n z^n = (1-z)^{-1/2}(1+z)^{1/4}(z-3+2^{3/2})^{1/8}(z-3-2^{3/2})^{1/8}, \qquad (1.15)$$

where $z = e^{-4J/kT}$. From Darboux's first theorem, Ninham (1963) obtained the asymptotic form of the coefficients a_n in the first and second Darboux approximations (i.e. to leading order and to order n^{-1}). The comparison is shown in Table 1.1. From the table it can be seen that Darboux's theorem gives an asymptotic form of considerable accuracy. Nevertheless, two remarks should be made. First, the function M_0 given by (1.15) has a series expansion whose coefficients are rapidly dominated by the closest singularity to the origin, and, secondly, it is much simpler to obtain an asymptotic representation of the series coefficients from the function than to extract information about the function from a knowledge of even many coefficients. We illustrate this more clearly in the discussion of the ratio method later in this section.

Table 1.1 Comparison between actual coefficients of the series expansion for M and the first and second Darboux approximations. (Taken from Ninham (1963)).

Order of coefficient of z^n, n	Coefficient in Darboux approximation		Actual coefficient
	1st approximation	2nd approximation	
6	670	700	714
7	3 300	3 410	3 472
8	16 550	17 020	17 318
9	84 830	86 520	88 048

1.5 Darboux's second theorem

To determine the asymptotic form of the coefficients of a function with more than one singularity on its circle of convergence, we turn to Darboux's second theorem. This may be stated as follows.

Suppose that a function $F(z)$ is analytic in the closed disc $|z| \leq 1$, and has a finite number of singularities $e^{i\phi_1}, e^{i\phi_2}, e^{i\phi_3}, \ldots, e^{i\phi_l}$, where $e^{i\phi_\alpha} = e^{i\phi_\beta}$ for $\alpha \neq \beta$, on the circle $|z| = 1$. Then if

$$F(z) = \sum_{\nu=0}^{\infty} c_\nu^{(k)}(1 - ze^{i\phi_k})^{\alpha_k + \nu\beta_k} = \sum_{n=0}^{\infty} a_n z^n, \quad k = 1, 2, \ldots, \qquad (1.16)$$

in the vicinity of $e^{i\phi_k}$, where $\beta_k < 0$, the expression

$$\sum_{\nu=0}^{\infty} \sum_{k=1}^{l} c_\nu^{(k)} \frac{(\alpha_k + \nu\beta_k)!}{n!} (-e^{i\phi_k})^n [(\alpha_k + \nu\beta_k - n)!]^{-1} \qquad (1.17)$$

furnishes an asymptotic expansion for the coefficient a_n in the following sense: if Q is an arbitrary positive number, and a sufficiently large number of terms in the sum over ν in (1.17) is taken, we obtain an expression that approximates the coefficient in question with an error $O(n^{-Q})$. That is, the infinite sum over ν is *not* claimed to be convergent. Szegö (1959) proved this theorem for a particular choice of function F, but his proof may be readily extended to any function satisfying the conditions stated above.

To illustrate the theorem, consider the function

$$f(x) = (1-x)^{-1/2}(1+x)^{-1/2} = \sum_{n=0}^{\infty} a_n x^n, \qquad (1.18)$$

series has recently been extended to 20 terms by Guttmann (1989), and is

$$C(x) = 1 + 6x + 30x^2 + 138x^3 + 618x^4 + 2730x^5 + 11\,946x^6 + 51\,882x^7$$
$$+ 224\,130x^8 + 964\,134x^9 + 4\,133\,166x^{10} + 17\,668\,938x^{11}$$
$$+ 75\,355\,206x^{12} + 320\,734\,686x^{13} + 1\,362\,791\,250x^{14}$$
$$+ 5\,781\,765\,582x^{15} + 24\,497\,330\,332x^{16} + 10\,367\,396\,7882x^{17}$$
$$+ 438\,296\,739\,594x^{18} + 185\,123\,137\,6374x^{19}$$
$$+ 7\,812\,439\,620\,678x^{20} + \ldots .$$

In Table 4.1 we show poles and residues of the tridiagonal Padé approximants to the logarithmic derivative of $C(x)$. There is clearly a strong temptation to conclude, as has been done in the past, that $z_c = 0.24088$ and $\gamma \approx 1.333$. From here, it is only a short step to the suggestive conjecture that $\gamma = \frac{4}{3}$. Indeed, for many years this was believed to be an exact result, and it was only in 1982 that Nienhuis was able to show that $\gamma = \frac{43}{32} = 1.34375$, which differs from the previously assumed value by less than 1%. How can this behaviour be explained, and more particularly, can we ensure that such incorrect conclusions are not drawn? (In fairness, we remark that the 20-term series is several terms longer than that available to the pioneers who conjectured that $\gamma = \frac{4}{3}$.)

Looking more closely at Table 4.1, we see first that, as N increases, there is a tendency for estimates of both z_c and γ to increase for N up to about 7. This tendency is by no means a monotonic trend, but is fairly clear. The bulk of the approximants with $N \leq 8$ are clustered around the

Table 4.1 D log Padé approximants to the chain-generating function of the triangular-lattice self-avoiding walk.

	$[N-1/N]$		$[N/N]$		$[N+1/N]$	
N	Pole	− Residue	Pole	− Residue	Pole	− Residue
4	0.24017	1.2926	0.24029	1.2971	0.24052	1.3062
5	0.23993	1.2880*	0.24061	1.3109	0.24144	1.4263
6	0.24070	1.3169	0.24079	1.3234	0.24083	1.3276
7	0.24090	1.3357	0.24087	1.3318	0.24088	1.3345
8	0.24088	1.3330*	0.24088	1.3333*	0.24088	1.3334*
9	0.24088	1.3336*	0.24088	1.3332*	complex	complex
10	0.24087	1.3327*				

* Defective approximant.

values cited above. Those marked with an asterisk are *defective*. That is, there is a pole–zero pair closer to the origin than the physical singularity. To make this clearer, for the [8/8] approximant we have a root of the denominator at $z = z^* = -0.13311367$ with residue 3.8729867×10^{-8}, while the numerator has a root at the same value of z (to the accuracy quoted), with residue 7.8945549×10^8. This means that, loosely speaking, the [8/8] approximant differs from the [7/7] approximant by a factor $z - z^*$ in both the numerator and denominator. The extra two series coefficients have not been used to construct a more accurate representation of the function, but rather to introduce a spurious pole–zero pair, which virtually cancel one another. This then gives a false impression of convergence, and must be guarded against by a careful examination of the pole/zero distribution of the approximants.

Given that most exponents of interest in critical phenomena are in the range 0.1–10.0, Hunter and Baker (1973) suggested the *ad hoc* procedure that poles be deemed defective if the absolute value of the residue is less than 0.003 and lies approximately inside the physical disc. One occasionally encounters a closely adjacent pair of poles in the vicinity of the critical point, and this too signals that caution must be exercised in accepting the approximants. The precise origin of such defective approximants can be seen as follows. Given an approximant $[N-1/D-1]$, if the higher-order approximant $[N/D]$ is related to $[N-1/D-1]$ by $[N/D] = [N-1/D-1](1-\alpha x)/(1-\beta x)$ then there exists an infinite family of solutions for arbitrary $\alpha = \beta$. If α is very close, but not equal, to β then the linear systems defining the polynomials in $[N/D]$ will be nearly singular, the residue at the pole $x = 1/\beta$ will be very small, and clearly we have no further information on the function—that is, the $[N/D]$ approximant still represents the function by an $[N-1/D-1]$ approximant, multiplied by an irrelevant factor $(1-\alpha x)/(1-\beta x)$.

Thus the correct interpretation of a Padé table is a non-trivial exercise, requiring careful consideration of defective approximants, the decomposition of Padé tables into blocks of essentially stable approximants (due to defects), and an identification of the scatter between distinct blocks of the Padé table. Only then can an assessment of the probable accuracy in estimates of the critical parameters be made.

This assessment should also utilize a quite general error analysis that has been given by Hunter and Baker, and is particularly interesting since it shows how errors in different critical parameters are related to one another, and shows why, and to what extent, the accuracy of critical-point estimates is better than that of critical-exponent and critical-amplitude estimates. Their analysis, with minor changes in notation, is given below, and generalizes the specific error analysis of the ratio method given at the end of Section 2.

$assign sqpols.dat for005	(this assigns the input file to unit 5)
$assign sqpols.out for006	(this assigns the output file to unit 6)
$run newgrqd	(this runs the previously compiled program)

On the following pages we show the input data, the transcript of the screen session and a small sample of the output produced. We seek first- and second-order unbiased differential approximants. Only inhomogeneous approximants are sought, with the degree of the inhomogeneous polynomial ranging from 1 to 8.

In order to present these data in a more accessible form, they are summarized and tabulated by the program TABUL. This program is also written in Fortran. To use this program with the data produced by the previous run, we proceed as shown. Again, a VMS environment is assumed. The input file to this program is the output file from the previous program, sqpols.out.

$ ty sqpols.dat (INPUT DATA FOR NEWGRQD)

```
square lattice polygons
 0 0 0
26
1.0
2.0
7.0
28.0
124.0
588.0
2938.0
15268.0
81826.0
449572.0
2521270.0
14385376.0
83290424.0
488384528.0
2895432660.0
17332874364.0
104653427012.0
636737003384.0
3900770002646.0
24045500114388.0
149059814328236.0
928782423033008.0
5814401613289290.0
36556766640745936.0
230757492737449636.0
1461972662850874916.0
9293993428791901042.0
    1    2    3   14                                1    8

 9
```


TRANSCRIPT OF SCREEN SESSION RUNNING NEWGRQD

```
$ assign sqpols.dat for005
$ assign sqpols.out for006
$ run newgrqd
FORTRAN STOP
```

11.2 ANALYSE and NEVBARB to calculate and extrapolate ratios

The next two programs take as input a series and then form ratios, linear extrapolants, unbiased exponent estimates and biased exponent estimates as defined by (2.4), (2.9), (2.11) and (2.12) respectively. The option of transforming the series by an Euler transformation (see Section 8) is also given. The data-deck make-up is as shown in the following screen transcript. The first record is a title (up to 80 characters). The second record (for ANALYSE) gives the number of series coefficients minus 1 (for a series starting with a constant this is the maximum power of the expansion variable). The series coefficients then follow, and the data file is terminated by a blank record followed by a record containing a negative number. The interactive program ANALYSE assumes this data is in a file called *textin.dat* and writes its output to a file called *textout.dat*. The parameter "mu" is the reciprocal of the critical-point estimate (needed if the series is to be Euler-transformed, and also for biased exponent estimates). If an Euler transformation $y = x(1+\alpha)/(1+\alpha x/x_c)$ is required, the parameter α as defined in Section 8 near (8.4) is then requested. As explained in Section 8, α should be chosen as small as possible. Finally, a choice of Levin transformation (t, u or v) is requested. We have found u to be the best choice in the overwhelming majority of cases.

Sample output is shown following the transcript of the screen session.

The data-deck make-up for NEVBARB is similar, except that it is not interactive, and so the second record of input data contains, in order, the maximum power of the expansion variable, a code = 0 for no Euler transformation, (otherwise code = 1 for an Euler transformation), the estimate of mu (the reciprocal of the critical point), and finally the value of α to be used in the Euler transformation.

Sample output from this program is also shown.


```
$ ty textin.dat     (INPUT DATA FOR ANALYSE)

square lattice polygons
26
1.0
2.0
7.0
28.0
124.0
588.0
2938.0
15268.0
81826.0
449572.0
2521270.0
14385376.0
83290424.0
488384528.0
2895432660.0
17332874364.0
104653427012.0
636737003384.0
3900770002646.0
24045500114388.0
149059814328236.0
928782423033008.0
5814401613289290.0
36556766640745936.0
230757492737449636.0
1461972662950874916.0
9293993428791901042.0

-1
```



```
$ run analyse
Default mu of 1  [Y] ?
n
Value of mu is ?
6.9598803
Apply Euler transformation to series [Y] ?
n
Enter levin transform type (t,u,v)  ?
u
```

TRANSCRIPT OF SCREEN SESSION RUNNING ANALYSE. USER RESPONSES UNDERLINED.