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A recurrence technique for confluent singularity analysis of power series

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Abstract. A generalisation of the recurrence method of series analysis is developed which permits the analysis of power-law confluent singularities in a function from its expansion in a power series. This method yields directly critical points and associated exponents for each element of an array of Kth-order, inhomogeneous, *differential equation approximants* $[M_0, M_1, \ldots M_K; L]$. Biased approximants are also discussed. Tests are presented which show that the method can be superior to the Dlog Padé approximant for determining the dominant critical exponent in a function known to have confluent singularities, and can yield good approximations for the leading confluent exponent. An application to the problem of determining correction-to-scaling exponents in 3D spin-∞ Ising models yields results in agreement with other studies.

1. Introduction

One of the fundamental tasks of series analysis is to predict the analytical and singular structure of a function $\psi(z)$, given the first several terms in its series expansion,

$$\psi(z) = \sum_n c_n z^n. \tag{1}$$

Techniques for analysing such series have diverse applications throughout theoretical physics (see, for example, Van Dyke 1974) and have been of particular importance in the theory of critical phenomena (see, for example, Gaunt and Guttmann 1974, Hunter and Baker 1973).

Our understanding of critical phenomena has increased considerably in recent years with the development of renormalisation group theory (Wilson and Kogut 1974, Domb and Green 1976 and references therein). One of the more striking predictions of the theory is that critical point singularities generally have an intrinsic *confluent* power-law nature (Wegner 1972). For example, thermodynamic quantities, such as the magnetic susceptibility $\chi(z)$, with z an appropriate temperature variable, should behave close to a critical point as

$$\psi(z) \underset{z \to z_c}{=} A_0(z) + A_1(z)|z - z_c|^{-\gamma_1} + A_2(z)|z - z_c|^{-\gamma_2} + \ldots \tag{2}$$

where $A_0(z)$, $A_1(z)$, $A_2(z)$, ... are regular at z_c, and $\gamma_1 > \gamma_2 > \ldots$.

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Such confluent singularities have been found rigorously in the triangular lattice Ising model with triplet-spin interactions (Baxter and Wu 1973, 1974, Baxter 1974, Joyce 1975a, b); by series analysis for spin-s Ising models (Saul *et al* 1975, Camp and Van Dyke 1975, Camp *et al* 1976); and in generalised spin models (Golner and Riedel 1976, Van Dyke and Camp 1975). However, non-analytic confluent corrections are absent in the 2D spin-$\frac{1}{2}$ Ising model (Barouch *et al* 1973), and all presently available series evidence (Sykes *et al* 1972) suggests their absence in the 3D spin-$\frac{1}{2}$ Ising model as well. Confluent singularity structure of the form (2) had previously been predicted by thermodynamic arguments for systems lacking the symmetry properties of spin-systems (see Rehr and Mermin 1973 and references therein).

The interference from confluent singularities can render ineffective conventional series analysis techniques, e.g. the Dlog Padé approximant, which are best suited for functions with strong, isolated, power-law singularities. This has led to the development of several techniques (Baker and Hunter 1973, Moore *et al* 1974, Camp and Van Dyke 1975), all inherently non-linear, for resolving such confluent singularities.

The main purpose of this article is to describe a generalisation of the 'recurrence method of series analysis' (Guttmann and Joyce 1972, Joyce and Guttmann 1973, hereafter referred to as I and II, respectively), which permits a direct analysis of such confluent power-law singularities from a given series. In addition we discuss how 'biased' estimates can be obtained, and we have incorporated in our analysis all of the possible generalisations of the recurrence method mentioned in I and II. All of these improvements have been implemented into a single FORTRAN program. The generalisation to 'inhomogeneous approximants' has also been discussed recently by Hunter and Baker (1979) and Fisher and Au-Yang (1979).

In brief, the recurrence method is based on fitting the series coefficients in equation (1) to a linear recurrence relation or, equivalently, to the polynomial coefficients of a Kth-order differential equation. These *differential equation approximants* (or simply 'differential approximants' in the terminology of Fisher) implicitly define approximate 'representations' $\psi_{M,L}(z)$, termed *integral approximants* by Hunter and Baker, of the desired function. Critical points and critical exponents are obtained using standard techniques from the theory of differential equations; it is not necessary to fit the amplitudes of singularities as in other procedures. By choosing the appropriate degree K, these approximants can often provide a better representation of the singular structure of a function than is possible with other methods. Indeed, tests of the recurrence method on functions with isolated singularities have shown that it is often superior to any other for a variety of test functions, with first-order inhomogeneous approximants usually performing better (Hunter and Baker 1979) than homogeneous second-order approximants (Guttmann 1975). Since many of the currently used methods of series analysis (ratio method, Neville extrapolants, Padé approximants, Dlog Padé approximants, etc) are special cases (Hunter and Baker 1979), our generalised recurrence method should have a wide applicability. An application to the analysis of spectral densities has already been made by Wheeler *et al* (1974). Furthermore, the inherent power and simplicity of the theory permits many additional refinements and generalisations. One such generalisation to the case of *partial differential approximants* for functions of two variables has been developed by Fisher and co-workers (Fisher 1977, Fisher and Kerr 1977, Fisher and Au-Yang 1979).

The remainder of this paper is organised as follows. In § 2 we give a detailed discussion of the recurrence method, together with our generalisation for confluent singularity analysis. The method is illustrated in § 3 for test functions formed from

hypergeometric functions, and for the internal energy series of the triplet-spin Ising model. Finally, in § 4 the method is applied to the determination of the Wegner correction to scaling exponent Δ_1 in the spin-∞ Ising model, and compared with other methods of confluent singularity analysis.

2. Recurrence method of series analysis

As descriptions of the recurrence method have appeared previously only in abbreviated form, we begin a full review of the method. Our discussion parallels that given in I and II but includes explicitly all of the possible generalisations and refinements noted there. For additional discussion, particularly with respect to first-order inhomogeneous approximants, we refer the reader to the papers of Hunter and Baker (1979) and Fisher and Au-Yang (1979).

2.1. Recurrence relations

We consider a function $\psi(z)$, analytic in some disc $|z|<r_0$, for which the first $\bar{N}$ terms of its Taylor expansion about the origin, equation (1), are known exactly. For definiteness we assume $c_0 \neq 0$, and set $c_{-n} \equiv 0 (n>0)$. The starting point of the recurrence method is to force the leading $N+1$ coefficients $c_0, c_1, \ldots, c_N (N \leqslant \bar{N})$ to satisfy exactly an $(M+1)$-term linear recurrence relation,

$$R_{\boldsymbol{M},L}[c_n] \equiv \sum_{i=0}^{K} \sum_{j=0}^{M_i} Q_{i,j}(n-j)^i c_{n-j} = P_n \qquad (n \geqslant 0). \tag{3}$$

Each recurrence relation is determined unambiguously by a set of integers (see also equation (16))

$$[M_0, M_1, \ldots, M_K; L] \equiv [\boldsymbol{M}, L] \tag{4}$$

with $K \geqslant 0$, $M_i \geqslant -1$ $(i=0, \ldots, K)$, $L \geqslant -1$; the definitions $Q_{i,-j} = P_{-j} \equiv 0 (j>0)$; and the normalisation condition, $Q_{K,0} \equiv 1$. The number of terms in the recurrence relation is set by

$$M = \max\{M_i, i=0, \ldots, K\}. \tag{5}$$

The coefficients $\{Q_{i,j}, P_j\}$ are determined by solving the system of linear equations (3), $\{R_{\boldsymbol{M},L}[c_n] = P_n \ (n=0, \ldots, N)\}$, provided a solution exists, where

$$N = \Sigma + K + L - N_b \tag{6}$$

$$\Sigma \equiv \sum_{i=0}^{K} M_i \tag{7}$$

and N_b is the number of additional independent constraints on the coefficients $\{Q_{i,j}, P_j\}$ one chooses to impose (§ 2.6).

Often we shall restrict our considerations to *homogeneous* recurrence relations, for which $P_j \equiv 0$ (or, equivalently, $L=-1$). These are designated simply by

$$\boldsymbol{M} \equiv [M_0, M_1, \ldots, M_K] \equiv [M_0, M_1, \ldots, M_K; -1]. \tag{8}$$

In this case equation (2.4) becomes

$$N = \Sigma + K - 1 - N_b \tag{9}$$

and we deduce from $R_{\boldsymbol{M}}[c_0] = 0$ that $Q_{0,0} = 0$.

By repeating the above procedure for all $[\boldsymbol{M}, L]$ for which $N \leq \bar{N}$ with K fixed, one obtains a $(K+2)$-dimensional array of recurrence relations (3) for the coefficients c_n; similarly, for homogeneous recurrence relations one obtains a $(K+1)$-dimensional array. This is a natural generalisation of the Padé table.

2.2. Approximate representations

Once the coefficients $\{Q_{i,j}, P_j\}$ defining the recurrence relation (3) have been determined, one can generate additional series coefficients $\tilde{c}_n (n > N)$ by recurrence, successively solving

$$R_{\boldsymbol{M},L}[\tilde{c}_n] = 0 \qquad (n > N) \tag{10}$$

for $\tilde{c}_n$. In this way a recurrence relation $[M_0, M_1, \ldots, M_K; L]$ together with the known series coefficients $c_n (n = 0, \ldots, N)$ implicitly define a representative function $\psi_{\boldsymbol{M},L}(z)$, whose series expansion agrees with equation (1) *at least* through terms of order N:

$$\psi(z) = \psi_{\boldsymbol{M},L}(z) + O(z^{N+1}). \tag{11}$$

Thus the recurrence method yields implicitly an array of approximate representations of the function $\psi(z)$ (*integral approximants*). Additional representations of $\psi_{\boldsymbol{M},L}$ will be discussed in § 2.7.

We remark that this procedure also provides a mathematical tool for extending sequences of numbers with complex internal regularities, or for deducing exact recurrence relations, as in the theory of special functions.

2.3. Differential equation approximants

It is readily verified that the function $\psi_{\boldsymbol{M},L}(z)$ constructed above is a solution of a linear, inhomogeneous, Kth-order differential equation

$$\mathcal{L}_{\boldsymbol{M},L}\psi_K(z) \equiv \sum_{i=0}^{K} Q_i(z)\Delta^i \psi_K(z) = P(z) \qquad \Delta \equiv z\, \mathrm{d}/\mathrm{d}z \tag{12}$$

which we term a *differential equation approximant.* The polynomial coefficients in equation (12) are

$$Q_i(z) = \sum_{j=0}^{M_i} Q_{i,j} z^j \tag{13}$$

and the driving term is

$$P(z) = \sum_{j=0}^{L} P_j z^j. \tag{14}$$

By inspection, $K = 0$ approximants correspond to standard $[L/M_0]$ Padé approximants (Baker 1974). Similarly, $K = 1$ approximants are equivalent to $[M_0 - 1/M_1]$

Dlog Padé approximants (Baker 1961),

$$\frac{\mathrm{d}\log\psi_K(z)}{\mathrm{d}z}=\left(\sum_{j=1}^{M_0}Q_{0,j}z^{j-1}\right)\left(\sum_{j=0}^{M_1}Q_{1,j}z^j\right)^{-1}. \tag{15}$$

In view of this correspondence, the notation (Fisher and Au-Yang 1979, Hunter and Baker 1979)

$$[L/M_0; M_1, \ldots, M_K]\equiv[M_0, M_1, \ldots, M_K; L] \tag{16}$$

has been proposed, though a reversed ordering, as in $[M_1, \ldots, M_K; L/M_0]$, might sometimes be preferable.

The use of the differential operator $\Delta = z(\mathrm{d}/\mathrm{d}z)$, rather than $(\mathrm{d}/\mathrm{d}z)$, considerably simplifies the structure of the recurrence relations. This form is also naturally suited (Hunter and Baker 1979) for obtaining Neville extrapolants with the method. A possible drawback is that the point $z = 0$ is generally forced to be a *regular singular point* of (12). This constraint can be removed by constructing recurrence relations from a differential equation written in 'standard form',

$$\sum_{l=0}^{K}W_l(z)\,\mathrm{D}^l\psi_K(z)=P(z), \qquad \mathrm{D}\equiv\mathrm{d}/\mathrm{d}z, \tag{17}$$

where $W_l(z)=\Sigma_{j=0}^{M_l}W_{l,j}z^j$ are polynomials of degree M_l. Our preliminary investigations with such recurrence relations did not reveal any advantage over those discussed above, but this remains a topic for further study.

We note that if equation (12) is written in standard form the polynomials $W_l(z)$ are $O(z^l)$ and given by

$$W_l(z)=z^l\sum_{i=l}^{K}\bar{S}_i^{(l)}Q_i(z) \tag{18}$$

where $\bar{S}_i^{(l)}$ are Stirling numbers of the second kind.

2.4. Analysis of critical points and critical exponents

The singular behaviour of the approximants $\psi_{M,L}(z)(K\geqslant 1)$ can be determined by applying standard techniques from the theory of differential equations (Whittaker and Watson 1927, Ince 1927) to the differential equation approximants (12). Our treatment below is not intended to be exhaustive. We emphasise at the outset that it is not necessary to evaluate the integrals $\psi_{M,L}$ to determine either the critical points or the corresponding critical exponents; however, a suitable integration is required to obtain critical amplitudes (see § 2.7).

The singular points z_i of the 'general solution' to the differential equation (12) are in general given by the M_K zeros of the polynomial $Q_K(z)$, $z=z_i$ $(i=1,\ldots,M_K)$, together (usually) with points $z_0=0$ and $z_\infty=\infty$, which we examine separately.

Let us first consider the case in which these zeros are distinct and in which the polynomials $Q_i(i=0,\ldots,K)$ have no common factors. These conditions usually prevail in most numerical calculations. Under these circumstances the zeros z_i are *regular singular points* of the differential equation. The K critical exponents defined at each point z_i $(\alpha_i, \beta_i, \ldots)$ are associated with the independent solutions $\psi_i(z)=A_i(z)|z-z_i|^{\alpha_i}$ of the homogeneous differential equation and are determined by the

indicial equation at z_i. In the present case there is only a single non-vanishing exponent given by

$$\alpha_i = K - 1 - Q_{K-1}(z_i)/z_i Q'_K(z_i) \tag{19}$$

while the remaining $K-1$ exponents are identically zero. Thus the general solution (Ince 1927) has the form

$$\psi_{M,L}(z) \underset{z \to z_i}{=} A_i^{(z)} |z - z_i|^{\alpha_i} + B(z) \tag{20}$$

where $A_i(z)$ is analytic at z_i, and $B(z)$ is analytic ($K=2$; $K=1, L \geqslant 0$), or contains analytic functions together with powers of logarithms ($K>2$), or vanishes ($K=1$, $L=-1$). Thus the recurrence method is naturally suited for functions with cusp singularities ($\alpha_i > 0$) or with weak, divergent non-factorisable singularities.

2.5. Confluent singularity analysis

Let us now consider a function with a finite number N_c of confluent power-law singularities at a given point z_c, as in equation (2). We shall assume that no pair of the associated exponents differ by an integer and that none is a positive integer or zero. A differential equation which faithfully accounts for the singular structure in such a function must have degree $K \geqslant N_c$, with common zeros in all the polynomials $Q_j(z)$ with $j > K - N_c$. In particular, the conditions are that $Q_j(z) = O[(z-z_c)^{N_c+j-K}]$, or equivalently,

$$0 = Q_j(z_c) = Q'_j(z_c) = \ldots = Q_j^{(m)}(z_c) \qquad (j > K - N_c) \tag{21}$$

where $m = N_c + j - K - 1$. A point at which the confluence (21) holds is also a regular singular point of the differential equation (12). However, in this case the analysis of the critical exponents generally involves an indicial equation of degree N_c, rather than one as simple as in equation (19).

In the case of two confluent singularities, for example, z_c will be a double zero of $Q_K(z)$ and a single zero of $Q_{K-1}(z)$, $K \geqslant 2$. Thus, the indicial equation reduces to a form quadratic in the critical exponents,

$$(\alpha + 2 - K)(\alpha + 1 - K)\frac{z_c^2}{2} Q''_K(z_c) + (\alpha + 2 - K) z_c Q'_{K-1}(z_c) + Q_{K-2}(z_c) = 0. \tag{22}$$

From the two solutions of equation (22) one obtains estimates for the critical exponents α and β, for each approximant, while the remaining $K-2$ exponents, if any, are zero.

The result of this analysis is that the singular behaviour of $\psi_{M,L}(z)$ at z_c in this case ($N_c = 2$) is given by

$$\psi_{M,L}(z) \underset{z \to z_c}{=} A(z)|z - z_c|^{\alpha} + B(z)|z - z_c|^{\beta} + C(z) \tag{23}$$

where $A(z)$ and $B(z)$ are analytic at z_c and $C(z)$ is analytic ($K=3$; $K=2$, $L \geqslant 0$), or contains powers of logarithms ($K>3$), or vanishes ($K=2$, $L=-1$).

In practice the roots of $Q_K(z)$ determined by the recurrence relations (3) are seldom degenerate. However, *closely spaced zeros* in $Q_K(z)$ are then symptomatic of confluent singularities in $\psi(z)$. As the *derivative* coefficients in the indicial equation (22) are generally non-zero and smoothly varying near z_c, provided that the spacing between the pair is sufficiently small and no other zeros are nearby, we may expect that the solutions

of equation (22) at *either zero* will still yield good approximations of α and β. To see this consider the structure of a differential equation (12) as two critical points z_1 and z_2 coalesce. The polynomial $Q_K(z)$ must factor as $(z-z_1)(z-z_2)\ldots(z-z_K)$, so that $Q'_K(z_1 \text{ or } z_2) = O(z_1 - z_2)$, which vanishes as $z_1 \to z_2$. Since the indicial equation (19) is valid for $z_1 \neq z_2$, one deduces that $Q_{K-1}(z_1 \text{ or } z_2) = O(z_1 - z_2)$ also. Thus the criterion (21) for the confluence of two singular points is satisfied with an error of $O(z_1 - z_2)$. Similarly, by substituting into the homogeneous differential equation the solution $\psi(z) = (z-z_c)^\alpha[1 + a_1(z-z_c) + \ldots]$, $z_c = z_1$ or z_2, one finds (cf equations (27)–(30)) that the critical exponent α satisfies an indicial equation of the form (22), but with coefficients differing only by terms containing $Q'_K(z_c)$ and $Q_{K-1}(z_c)$ which are $O(z_1 - z_2)$. Thus, barring identical exponents, the solution to the indicial equation (22) in the case of closely spaced singular points should yield 'effective exponents' which differ from the correct values by an amount of $O(z_1 - z_2)$. In any case, this procedure yields two estimates of each of the critical exponents and therefore provides a natural consistency check.

By a straightforward generalisation of these results we see that a solution with N_c confluent power-law singularities requires the determination of at least $N_c + 1$ polynomials $\{Q_i(z), P(z)\}$. Thus the procedure can become expensive in the number of exact series coefficients required. Also, for a limited number of exact coefficients, one is restricted to increasingly smaller-degree polynomials for increasingly larger K, but in compensation a larger number of approximants can be defined.

A similar analysis for the singular point $z_0 = 0$ generally yields K (or $K-1$ if $L = -1$) confluent power-law singularities. The analysis at $z_\infty = \infty$ can be more complicated. However, if $M_K = M$, z_∞ is also a regular singular point and a similar analysis holds. Also in this case one can usually establish a sum rule on all the critical exponents.

Finally, we note that it is possible to consider many other types of singularities within the present framework. For example, certain essential singularities are defined by the condition that $Q_K(z)$ has a double-zero at a point z_c where $Q_{K-1}(z_c)$ is non-zero. However, many singularities, such as fractional powers of logarithms, cannot be described in terms of a finite-order linear differential equation with polynomial coefficients.

2.6. Biased approximants

As in many other series analysis techniques, it is possible to obtain *biased* estimates of critical points and critical indices by fixing *a priori* the locations of one or more singular points, possibly together with one or more of the corresponding critical exponents.

In the present method singular points z_i with or without confluent singularities are easily specified by imposing the conditions that the polynomials $Q_i(z)$ have zeros of appropriate multiplicity (equation (21)). These constraints lead to additional *linear* equations which must be satisfied by the recurrence relation coefficients $\{Q_{i,j}\}$. For example, to fix the location of an isolated singularity, one sets

$$\sum_{j=0}^{M_K} Q_{K,j} z_c^j = 0. \tag{24}$$

Similarly three equations are needed to specify each singular point with two confluent power-law singularities, etc.

Critical exponents may be specified simply by forcing the indicial equation (equations (19), (22), or an appropriate generalisation if $N_c > 2$) to be satisfied exactly at a

specified singular point. This leads to a single additional linear equation for each specified critical exponent which must be satisfied by the coefficients $\{Q_{i,j}\}$.

Note that biasing the differential equation approximant reduces the number of series coefficients required to define a given approximant, such reduction being equal to the number N_b of additional equations satisfied by the coefficients $\{Q_{i,j}, P_j\}$,

$$N_b = N_s + 3N_d + N_\alpha \tag{25}$$

where N_s is the number of specified isolated singular points, N_d is the number of specified points with two confluent singularities, etc, and N_α is the number of specified critical exponents. Note that if z_c is complex, equation (24) yields two independent constraints, but z_c^* will also be a singular point if $\{Q_{i,j}, P_j\}$ are real.

2.7. Critical amplitudes

While the recurrence method does not yield direct estimates of the *critical amplitudes*, A_i in equation (2), these quantities are defined implicitly for a given approximant by the series coefficients c_n. The following procedure based on recurrence techniques yields these amplitudes without the necessity of numerical integration.

Let us define the critical amplitudes as the coefficients A_i of the normalised independent solutions $a_i(z - z_c)$ in the general solution of the differential equation (12) in the vicinity of a singular point z_c,

$$\psi_K(z) = \sum_{i=0}^{K} A_i a_i(z - z_c). \tag{26}$$

By means of recurrence relations similar to (3) one can generate series developments of these solutions to arbitrarily many terms; these recurrence relations are defined uniquely for a given approximant. The critical amplitudes are then obtained by matching successive solutions, moving away from the origin, as in the process of analytic continuation.

As an example, consider the closest singularity to the origin for a second-order homogeneous approximant. Let

$$a_l(z - z_c) = \sum_{j=0}^{\infty} a_{l,j}(z - z_c)^{\alpha_l + j} \tag{27}$$

be the independent solutions to (12), with $a_{l,0} \equiv 1$ and $a_{l,-j} \equiv 0 (j > 0)(l = 1, 2)$. The coefficients $a_{l,j}$ in (27) satisfy a recurrence relation

$$R_M[a_{l,n}] = \sum_{i=0}^{K} \sum_{j=0}^{M_i} Q_{i,j}^{(l)} (\alpha_l + n - j)^i a_{l,n-j} = 0 \tag{28}$$

in which the coefficients $Q_{i,j}^{(l)}$ are simply related to the recurrence coefficients $Q_{i,j}$ constructed previously. Defining these coefficients implicitly in terms of polynomials $Q_{l,i}(z)$, as in equation (13),

$$Q_{l,i}(z) = \sum_{j=0}^{M_i} Q_{i,j}^{(l)} (z - z_c)^j \tag{29}$$

the correspondence is

$$Q_{l,2} = \frac{z^2 Q_2}{(z - z_c)^2} \qquad Q_{l,1} = \frac{z Q_1}{z - z_c} + \frac{z z_c Q_2}{(z - z_c)^2} \qquad Q_{l,0} = Q_0. \tag{30}$$

For the singularity closest to the origin there exists an intermediate point $|z_m| < |z_c|$ where both the expansion about the origin $\psi_M(z)$ and the newly constructed representation ψ_K are convergent. The critical amplitudes are then determined by the equations

$$\psi_M(z_m) = A_1 a_1(z_m - z_c) + A_2 a_2(z_m - z_c) \tag{31}$$

$$\psi'_M(z_m) = A_1 a'_1(z_m - z_c) + A_2 a'_2(z_m - z_c). \tag{32}$$

2.8. FORTRAN program

We have incorporated into a single FORTRAN program all of the generalisations of the recurrence method described above for treating up to two confluent singularities at each singular point ($z = 0$, excepted). Each desired differential equation approximant is specified by a set of integers, $[M_0, M_1, \ldots, M_K; L]$, together with, if desired, a set of auxiliary conditions and input data necessary to construct biased approximants. For each approximant, the program then determines the recurrence coefficients $\{Q_{i,j}, P_j\}$, the singular point locations, and the value of the associated critical exponent at each singular point given by the indicial equation (19). If two singular points are closely spaced (or identical, as in biased estimates) the program then determines two critical indices from the quadratic indicial equation (22), as discussed in § 2.5. The criterion presently used in the program to decide whether two singularities are closely spaced is that $|Q'_K(z_c)|$ be less than a small constant, typically set at 0·01 (the quantity $Q'_K(z_c) = O(\Delta z_c)$ where Δz_c is the spacing between nearly confluent singular points). The validity of this criterion may be checked by examining the singularity map. An alternative criterion would involve the *normalised* quantity $[Q'_K(z_c)/z_c Q''_K(z_c)] = O(\Delta z_c/z_c)$; however, this would necessitate a calculation of $Q''_K(z_c)$ at all singular points, confluent or not. The interpretation of results is discussed in previous parts of §§ 2 and 3. The program also has a provision for generating the series coefficients $\tilde{c}_n$ defining the approximants $\psi_{M,L}(z)$. Some additional details are mentioned by Guttmann (1975).

3. Test functions

In this section we carry out a number of tests of the method on functions known to have confluent, power-law singularities.

3.1. Hypergeometric-type test functions

We consider first functions formed from the sum and product of two hypergeometric functions. These test functions, labelled by the subscripts A and B, respectively, are defined as

$$\psi_A(z) = F(1, \tfrac{1}{2}, \tfrac{1}{4}; z) + F(1, \tfrac{1}{2}, \tfrac{3}{4}; z) \tag{33}$$

$$\psi_B(z) = F(1, \tfrac{1}{2}, \tfrac{1}{4}; z) F(\tfrac{1}{4}, \tfrac{1}{4}, 1; z), \tag{34}$$

and it is a straightforward matter to generate large numbers of series coefficients. The analytical structure of these functions (see, for example, Whittaker and Watson 1927) near the singular point at $z = 1$ is as follows:

$$\psi_A(z) \underset{z \to 1}{=} A_0(z) + A_1 |1 - z|^{-5/4} + A_2(z) |1 - z|^{-3/4} \tag{35}$$

$$\psi_B(z) \underset{z\to 1}{=} B_0(z)+B_1(z)|1-z|^{-5/4}+B_2(z)|1-z|^{-3/4}+B_3(z)|1-z|^{1/2} \tag{36}$$

where $A_i(z)$ and $B_i(z)$ are analytic at $z = 1$. The results of our analysis are summarised below.

3.1.1. Critical point location. We found the differential equation approximants (labelled RR in table 1) for $K = 2$ and 3 to be markedly superior to the Dlog Padé approximant ($K = 1$, labelled DP) for determining the location of the critical point at $z = 1$. Typical comparisons are given in table 1. The accuracies quoted refer to the logarithm of the relative error $\epsilon = -\log \Delta z_c/z_c$, and numbers in parentheses refer to the number of series coefficients in addition to c_0 (N in equation (9)) used to construct a given approximant. All of these tests were performed with unbiased, homogeneous, 'diagonal' $[M, M, \ldots, M]$ approximants.

Table 1. Comparative accuracies of estimates of the location of the critical point $z_c = 1$. The numbers quoted are values of $\epsilon(z_c) = -\log(\Delta z_c/z_c)$ and (in parentheses) N, the number of series coefficients used.

Test series	DP ($K = 1$)	RR ($K = 2$)	RR ($K = 3$)
A	1·8(4)	2·8(4)	
	3·2(10)	3·8(10)	
	4·0(18)	5·6(19)	
	4·6(28)	6·6(28)	
B	1·8(4)	2·7(4)	3·6(5)
	3·3(10)	4·2(10)	5·3(10)
	4·2(18)	5·2(19)	5·6(18)
	4·8(28)	6·0(28)	6·3(26)

3.1.2. Dominant critical exponent. Next we examine the estimates of the dominant critical exponent $\gamma_1 \equiv -\alpha_1$ (exact value $\gamma_1 = 1{\cdot}25$). We found both the Dlog Padé and the original recurrence method to give poor results for γ_1 (table 2, columns DP and RR). This is to be expected, considering the presence of the confluent singularities in these functions. For the longest series used, the performance of the Dlog Padé was slightly better than that with $K = 2$ approximants.

Table 2. Accuracies of estimates of the dominant critical exponent γ_1 (exact value 1·25). The numbers refer to $\epsilon(\gamma_1) = -\log(\Delta\gamma_1/\gamma_1)$ and (in parentheses) N, the number of series coefficients used.

Test series	DP ($K = 1$)	RR ($K = 2$)	GR ($K = 2$)	GR ($K = 3$)
A	1·5(10)	1·8(10)	2·3(13)	2·9(14)
	1·7(18)	1·4(13)	4·8(19)	6·2(18)
	1·9(28)	—	4·2(28)	5·1(26)
B	1·5(8)	1·9(7)	1·4(13)	2·5(14)
	1·9(18)	2·0(19)	3·1(19)	3·9(18)
	2·2(28)	1·7(28)	3·9(25)	4·5(26)

3.1.3. Confluent singularity analysis. In the columns labelled GR (for generalised recurrence method) of table 2, we list some *unbiased* estimates of the dominant critical exponent γ_1 as determined for a given approximant from the quadratic indicial equation. Comparison with columns DP and RR indicates that the confluent singularity analysis significantly improves the exponent estimates and provides good estimates even for rather short series.

Estimates of the leading confluent critical exponent $\gamma_2 \equiv -\alpha_2$ (exact value 0·75) are given in table 3. For $K = 2$ we find that γ_2 is reasonably well determined for test function A. This is remarkable, as a homogeneous differential equation of third order or greater is required to describe the singular structure of this function at $z = 1$. For test function B the accuracy with $K = 2$ approximants is much poorer, apparently as the result of interference of the weak confluent singularity with exponent $\gamma_3 = -\frac{1}{2}$. These results suggest that biased estimates or approximants with $K > 2$ may be advantageous if a function has more than two confluent singularities at a given point. This is borne out by examination of the $K = 3$ approximants. The above tests were all made with homogeneous, diagonal approximants.

Table 3. Accuracies of estimates of the confluent exponent γ_2 (exact value 0·75). The numbers refer to $\epsilon(\gamma_2) = -\log(\Delta\gamma_2/\gamma_2)$ and (in parentheses) N, the number of series coefficients used. Unbiased estimates are designated by a superscript U. In the biased estimates: I, $z_c = 1{\cdot}0$; II, $z_c = 1{\cdot}0$, $\gamma_1 = 1{\cdot}25$.

Test series	GR^U ($K=2$)	GR^U ($K=3$)	GR^I ($K=2$)	GR^I ($K=3$)	GR^{II} ($K=2$)	GR^{II} ($K=3$)
A	1·7(13)	2·0(14)	3·0(10)		3·3(9)	
	2·7(19)	6·7(18)	3·8(19)		4·7(18)	
	3·3(28)	5·7(26)	3·5(25)		3·7(24)	
B	0·8(13)	1·5(14)	1·3(10)	2·4(11)	1·5(9)	2·9(10)
	1·1(19)	2·4(18)	1·8(19)	3·4(19)	2·2(18)	4·7(18)
	1·7(28)	3·3(26)	2·3(28)	5·5(27)	2·7(27)	5·1(26)

3.1.4. Biased approximants. The remaining columns in table 3 illustrate the substantial improvement in the estimates of γ_2 when the approximants are biased. We consider two cases: (i) when the critical point $z = 1$ is specified, or (ii) when both $z = 1$ and $\gamma_1 = 1{\cdot}25$ are specified. Note that for test function A, γ_2 is determined quite well with $K = 2$ approximants, while for test function B the $K = 3$ approximants are significantly better.

Finally, to determine the stability of these biased estimates, the specified critical parameters were varied slightly from their exact values (figure 1). We observe that the behaviour of the dominant exponent γ_1 is much more stable than is γ_2. Note too that a small deviation of a critical point location or an exponent from its exact value dramatically increases the scatter among the various estimates. This suggests a way of obtaining accurate estimates when the precise singular point location is not known, which we will exploit in the next section.

3.2. Triplet-spin Ising model

As a third example we have performed an analysis parallel to that above for the internal

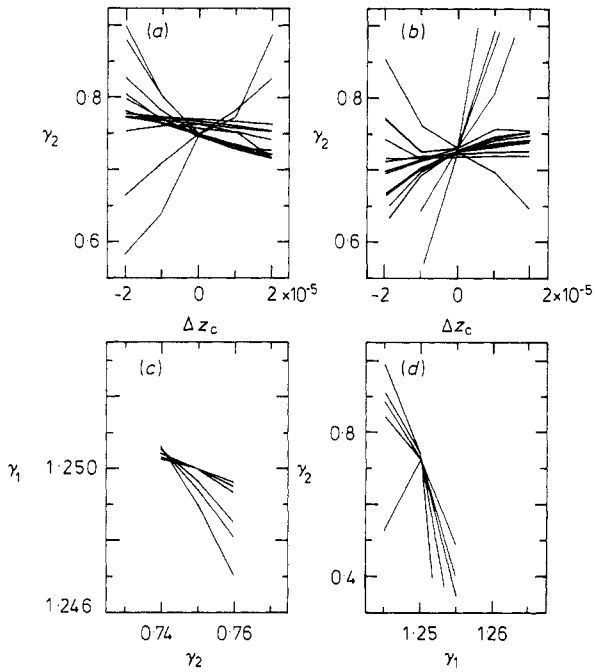

Figure 1. Stability of biased estimates with respect to a small change in z_c [parts (*a*) and (*b*) for ψ_A and ψ_B, respectively]; γ_2, part (*c*); and γ_1, part (*d*).

energy series $U(u)$ of the triplet-spin Ising model on a triangular lattice. The zero-field free energy $A(T)$ for this model is exactly soluble (Baxter and Wu 1974, Baxter 1974) and its analytic properties have been investigated by Joyce (1975a,b), who showed that

$$A(T) = -2J + k_B T \ln\left[(1+u)^{-2}\, {}_2F_1\left(\frac{1}{2}, \frac{1}{6}; \frac{4}{3}; \frac{16u(1-u)^2}{(1+u)^4}\right)\right] \tag{37}$$

where $u \equiv \exp(-2J/k_B T)$. We have used this exact solution to generate a large number of series coefficients for the internal energy series (Joyce 1975a,b). It follows from (7) that the analytic behaviour of $U(u)$ near the critical point $u_c = 3 - 2\sqrt{2}$ is given by

$$U(u) = A_0(u) + A_1(u)|u - u_c|^{1/3} + A_2(u)|u - u_c|^{5/3} \tag{38}$$

where $A_0(u)$, $A_1(u)$ and $A_2(u)$ are analytic functions at $u = u_c$. Our analysis is briefly summarised below.

3.2.1. Unbiased approximants. As in the previous examples, the unbiased differential equation approximants with $K = 2$ and 3 were found to be markedly superior to the Dlog Padé approximants ($K = 1$) in determining the location of the critical point. With about 20 series coefficients these approximants gave values of $\epsilon(u_c) = -\log(\Delta u_c/u_c)$ of 2·0, 5·4 and 6·5 for $K = 1$, 2 and 3, respectively.

The estimates of the dominant critical exponent were also striking. The estimates for the $K = 1$ approximants decayed very slowly toward *zero*, a value appropriate to the analytic part of U! Even with 40 series coefficients the exponent estimates were about $-0{\cdot}1$. By comparison the exponent estimates for $K = 2$ and $K = 3$ approximants were $\alpha_1 = 0{\cdot}3340$ and $0{\cdot}3337$, respectively, using only 16 series coefficients. The poor

performance of the homogeneous $K = 1$ approximants is to be expected for this class of function, as discussed in §§ 2.4 and 2.5. Interestingly, for sufficiently high degree approximants a nearly degenerate pair of zeros in Q_K was indicated by approximants of orders $K = 1$, 2 and 3.

3.2.2. Biased approximants. Next, biased estimates of exponents were obtained by specifying the position of the critical point at $u_c = 3 - 2\sqrt{2}$ to be a double-zero of $Q_K(u)$. Some results are presented in tables 4 and 5. Clearly the two exponents are converging to $\frac{1}{3}$ and zero for the $K = 2$ approximants. This is a particularly interesting example as it shows that for $K = 2$ the two *dominant* contributions to the function are 'selected' by the method, even though one of these is analytic. From the discussion in § 2.5, a differential equation approximant of third order (or an inhomogeneous approximant of second order) is required to fit the singular structure of (38). Thus, with the $K = 3$ approximants the full structure of the function is revealed: the exponents are clearly converging to $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{5}{3}$. The behaviour is similar for biased estimates in which both u_c and the dominant exponent are specified.

Table 4. Biased estimates of the critical exponent α_1 (exact value $\frac{1}{3}$) for the internal energy series of the triplet-spin Ising model, with $u_c = 3 - 2\sqrt{2}$. The numbers quoted are $\epsilon(\alpha_1) = -\log(\Delta\alpha_1/\alpha_1)$ and (in parentheses) N, the number of series coefficients used.

DP ($K = 1$)	GR ($K = 2$)	GR ($K = 3$)
−0·2(9)	1·4(10)	2·3(11)
−0·1(15)	2·3(16)	3·2(15)
−0·1(21)	3·2(25)	4·8(27)

Table 5. Biased estimates of the confluent exponents $\alpha_2 = \frac{5}{3}$ or $\alpha_0 = 0$ (analytic term) for the internal energy series of the triplet-spin Ising model. In I, $u_c = 3 - 2\sqrt{2}$; in II, $u_c = 3 - 2\sqrt{2}$ and $\alpha_1 = \frac{1}{3}$. The numbers refer to $\epsilon(\alpha_0) = -\log\Delta\alpha_0$ *or* $\epsilon(\alpha_2) = -\log(\Delta\alpha_2/\alpha_2)$; those in parentheses refer to the number N of series coefficients used.

$GR^{I}(K = 2)$ $\epsilon(\alpha_0)$	$GR^{II}(K = 2)$ $\epsilon(\alpha_0)$	$GR^{I}(K = 3)$ $\epsilon(\alpha_2)$	$GR^{II}(K = 3)$ $\epsilon(\alpha_2)$
2·4(10)	2·9(9)	−1·8(11)	−1·4(10)
3·4(16)	4·1(15)	0·5(15)	1·5(14)
4·6(25)	5·1(24)	1·4(27)	1·3(26)

4. Spin-∞ Ising models

In this final section we discuss the application of the generalised recurrence method to the problem of determining the correction-to-scaling exponents for the spin-∞ Ising model on an FCC lattice. In addition, we compare the results with those obtained by other methods. The series expansions analysed here are high-temperature series of 12 terms for the zero-field susceptibility $\chi(z)$ and for the second moment of the spin–spin correlation function $M_2(z)$, where $z = J/3k_BT$. These series have been the object of

detailed analyses (Saul *et al* 1975, Camp and Van Dyke 1975, Camp *et al* 1976) based on several methods of confluent singularity analysis, including the generalised ratio method, the Baker–Hunter transformation, and the method of four-fits. In this respect these series represent interesting cases for quantitative comparisons of our method.

One of the difficulties of treating these series is their short length. Another is that none of the critical parameters is known exactly, although γ_1 for the susceptibility series is believed to be very close to 1·25. We have therefore attempted to determine the critical point and the corresponding critical indices by making biased estimates as discussed in the two previous sections. The other methods of confluent singularity analysis mentioned above are also biased. Specifically we obtain estimates for the leading confluent exponent γ_2 by fixing γ_1 and varying z_c as in figures 1(*a*) and (*b*). Since longer, fairly well-behaved susceptibility series are available for the spin-$\frac{1}{2}$ Ising model (Sykes *et al* 1972, McKenzie 1975) which give $\gamma_1 = \gamma = 1{\cdot}25^{+0{\cdot}002}_{-0{\cdot}005}$, we shall adopt for χ the values $\gamma_1 = 1{\cdot}250$ or 1·245. For the second moment series we use $\gamma_1 = \gamma + 2\nu = 2{\cdot}526$ or 2·520 based on the values $\gamma = 1{\cdot}250$ and $\nu = 0{\cdot}638^{+0{\cdot}002}_{-0{\cdot}008}$ (Camp *et al* 1976). For comparison the Baker–Hunter method requires a given value of z_c, and both the generalised ratio method and the method of four-fits fix γ_1 to determine γ_2.

Our results are summarised in figures 2(*a*) and (*b*), for representative $[M_0, M_1, M_2]$ approximants using between 9 and 11 series coefficients (the twelfth terms of these series both give erratic estimates which are not included). The overall consistency of these results is noteworthy and provides a rough estimate of the accuracy that is possible with the generalised recurrence method. Table 6 lists the values of the critical parameters in figures 2(*a*) and (*b*) for which the scatter among the various approximants is minimal. In comparison with our values of z_c between 0·095033 and 0·095042, the generalised ratio method for the χ series yielded $z_c = 0{\cdot}095043$ while the method of four-fits gave 0·095025 for χ and 0·09506 for M_2. Since the correction to scaling exponent is $\Delta_1 = \gamma_1 - \gamma_2$ we find that $\Delta_1 \simeq 0{\cdot}5$ (for fixed $\gamma = 1{\cdot}250$, $\gamma + 2\nu = 2{\cdot}526$) and $\Delta_1 \simeq 0{\cdot}55$ (for fixed $\gamma = 1{\cdot}245$, $\gamma + 2\nu = 2{\cdot}520$). These values are in rough agreement with the results of Saul *et al* for χ, $\Delta_1 = 0{\cdot}5 \pm 0{\cdot}05$ (method of four-fits); with those of

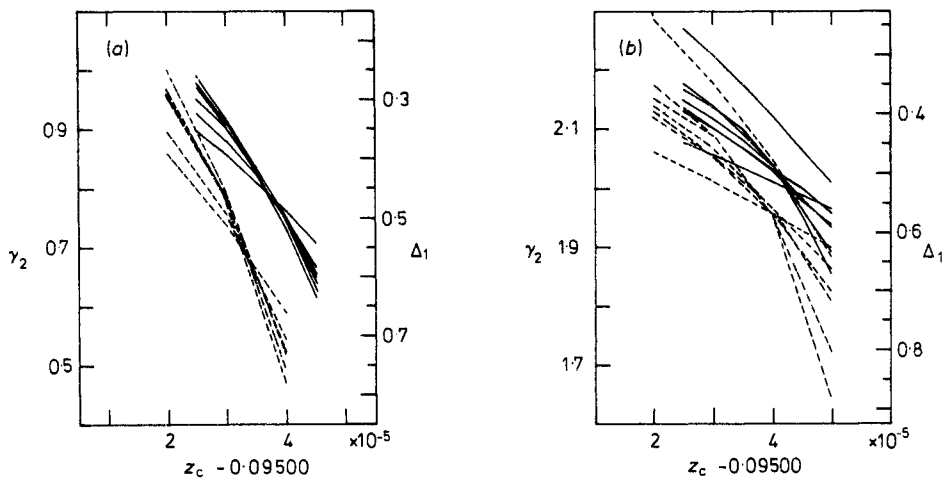

Figure 2. (*a*) Estimates of γ_2 for the susceptibility χ series plotted against a range of values of z_c. Straight line segments indicate estimates with $\gamma_1 = 1{\cdot}250$; broken lines $\gamma_1 = 1{\cdot}245$. The exponent $\Delta_1 = \gamma_1 - \gamma_2$. (*b*) Estimates of γ_2 for the second moment M_2 series plotted against z_c: straight lines indicate $\gamma_1 = 2{\cdot}526$; broken lines $\gamma_1 = 2{\cdot}520$.

Table 6. Confluent singularity analysis for the FCC spin-∞ Ising model. A superscript a denotes a fixed value.

Series	γ_1	γ_2	Δ_1	z_c
$\chi(z)$	$1{\cdot}250^a$	0·78	0·47	0·095 038
	$1{\cdot}245^a$	0·70	0·55	0·095 033
$M_2(z)$	$2{\cdot}526^a$	2·01	0·52	0·095 042
	$2{\cdot}520^a$	1·97	0·55	0·095 039

Camp *et al* for M_2, $\Delta_1 \simeq 0{\cdot}6 \pm 0{\cdot}1$ (Baker–Hunter method, and method of four-fits); and with the results of Camp and Van Dyke for χ, $\Delta_1 \simeq 0{\cdot}57$ (generalised ratio) and 0·55 (Baker–Hunter). These results indicate that with a limited number of coefficients the generalised recurrence method can yield accuracies roughly comparable to that of currently used confluent singularity analysis methods. While not an improvement on these methods the generalised recurrence method has the advantage that only linear equations are involved in the analysis and that a global representation of the function is obtained. On the other hand, this method does not yield critical amplitudes directly (see § 2.7). Since significant improvements should be possible with longer series, we hope these results will encourage others to extend the Ising model series.

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