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Inhomogeneous differential approximants for power series

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Abstract. Inhomogeneous differential approximants $[J/L; M]_{f(x)}$, $[\boldsymbol{J}/\boldsymbol{L}; \boldsymbol{M}, \boldsymbol{N}]_{f(x,y)}$, etc are defined for functions of one or more variables given as power series expansions, and some of their properties are exposed. The approximants are easily computable, and numerical studies are reported (for single-variable series) which demonstrate their utility in circumstances where the customary direct or logarithmic derivative Padé approximants (which are limiting cases) are inadequate.

1. Introduction

Given a function $f(x)$ defined through its power series

$$f(x) = \sum_{i=0}^{\infty} f_i x^i, \tag{1.1}$$

it is well known that a method of approximating the function on the basis of a restricted number of coefficients (say f_i for $i \leqslant I$), which is effective in a number of circumstances, is to calculate direct Padé approximants $[L/M]_f$ for $L+M \leqslant I$ (see e.g. Baker 1975, Fisher 1974). Likewise for a function of two variables, $f(x, y)$, with power series coefficients $f_{ii'}$, direct two-variable approximants, sometimes called Canterbury approximants, may be defined (Chisholm 1973, Chisholm and Roberts 1976). However, if, as in many practical applications, the function exhibits a branch point of the form

$$f(x) \approx A/(1 - x/x_c)^{\gamma}, \tag{1.2}$$

with γ positive and non-integral in the region of interest, direct Padé approximants to $f(x)$ cannot be effective and, in particular, they do not yield accurate estimates of the branch or 'critical' point x_c, of the exponent γ, or of the amplitude A. In such circumstances, following Baker (Baker 1975, Fisher 1974), recourse is normally had to the so-called 'D log Padé technique', in which the series for $D(x) = (\mathrm{d}/\mathrm{d}x) \log f(x)$ is formed from (1.1), and the Padé approximants $[L/M]_{D \log f}$ are calculated. This approach is often very effective and has had great successes.

However, the D log Padé technique does have a number of practical drawbacks. Whereas the ratio method of extrapolating series expansions, applicable when $f_i > 0$ (all i) (see e.g. Fisher 1974), is obviously invariant to alterations in the first few coefficients, $f_0, f_1, \ldots$, the D log Padé approach has no such invariance: indeed a transformation such as $\{f_0 \Rightarrow f_0 + 2,\ f_1 \Rightarrow f_1 - 3\}$ will typically result in a serious degradation in the accuracy of approximation. In addition, although not really independently, the D log

Padé method often performs poorly when the exponent γ is small (say $\gamma = 0{\cdot}1$ to $0{\cdot}4$). The reason, frequently, is simply that the representation (1.2) is inadequate, in that a significant constant or 'background' term B should be added to the right-hand side: in such a case one finds

$$D(x)=\frac{\mathrm{d}}{\mathrm{d}x}\log f(x)=\frac{-\gamma}{x-x_c}\left[1-\frac{B}{A}\left(1-\frac{x}{x_c}\right)^{\gamma}+\ldots\right]. \tag{1.3}$$

The leading pole may be accurately represented by an $[L/M]_{D\,\log f}$ approximant, but the branch cut implied by the correction term cannot be well approximated: if B/A is large and γ small, this can have a very strong effect.

Evidently, then, there is a need for a technique of approximation which can handle effectively functions such as

$$f(x)=A(x)/(1-x/x_c)^{\gamma}+B(x), \tag{1.4}$$

where $A(x)$ and $B(x)$ are analytic in the branch point or critical region $x \simeq x_c$: in particular, if $B(x)$ may be a low-order polynomial, it can clearly represent exactly changes in the first few coefficients f_i.

The situation for functions of two variables is analogous. The expected behaviour in the vicinity of a multisingular point (x_c, y_c), which replaces (1.2), for functions of two variables is

$$f(x, y)=\sum_{i,i'=0} f_{ii'}x^{i}y^{i'} \approx A\Delta\tilde{x}^{-\gamma}Z\left(\frac{\Delta\tilde{y}}{\Delta\tilde{x}^{\phi}}\right), \tag{1.5}$$

$$\Delta\tilde{x}=\Delta x-\Delta y/e_2, \qquad \Delta\tilde{y}=\Delta y-e_1\Delta x, \tag{1.6}$$

where $\Delta x = x - x_c$, $\Delta y = y - y_c \to 0$, while γ is the principal exponent and ϕ the 'cross-over exponent'; e_1 and e_2 are the slopes of the 'scaling axes', and $Z(z)$ is the 'scaling function' normalised, say, as $Z(0) = x_c^{\gamma}$ (Fisher 1977, Fisher and Kerr 1977). Again, direct two-variable or Canterbury approximants are not effective in representing $f(x, y)$ in the neighbourhood of a multisingular point or in estimating the crucial parameters x_c, y_c, γ, ϕ, e_1, e_2, A, and the function $Z(z)$. However, in this case it has been demonstrated (Fisher 1977, Fisher and Kerr 1977) that an effective method of approximation is to calculate 'partial differential approximants', $F_{\boldsymbol{L};\boldsymbol{M},\boldsymbol{N}}(x, y) = [\boldsymbol{L}; \boldsymbol{M}, \boldsymbol{N}]_f$, which satisfy an equation of the form

$$P_{\boldsymbol{L}}(x, y)F = Q_{\boldsymbol{M}}(x, y)\,(\partial F/\partial x)+R_{\boldsymbol{N}}(x, y)\,(\partial F/\partial y). \tag{1.7}$$

Here $P_{\boldsymbol{L}}$, $Q_{\boldsymbol{M}}$ and $R_{\boldsymbol{N}}$ are polynomials in x and y with coefficients $p_{ll'}$, $q_{mm'}$ and $r_{nn'}$ with labels drawn from sets $\boldsymbol{L} \supset (l, l')$, etc; the coefficients are to be chosen (by solving linear algebraic equations) so that the power series solution of (1.7), for appropriate boundary conditions, matches the known expansion in (1.5) as far as possible (i.e. on powers $x^k y^{k'}$ with (k, k') drawn from some maximal label set $\boldsymbol{K}$).

This approach has been used successfully (Fisher and Kerr 1977), but in practice one must again anticipate the presence of a background term $B(x, y)$ on the right-hand side of (1.5). Such a term will cause computational difficulties if it is relatively large or if γ is small. More generally, the amplitude A should be replaced by a function $A(x, y)$ analytic near (x_c, y_c), and one would like to allow $\Delta\tilde{x}$ and $\Delta\tilde{y}$ to be multiplied by functions $g(x, y)$ and $h(x, y)$, likewise analytical and non-vanishing in the multisingular region. As a matter of fact, it was the disturbing occurrence of such a background term in an ongoing study of two-variable functions representing magnetic bicritical behaviour (Fisher and Kerr 1977) that led us to the present considerations for functions of both one and two variables. (For the interested reader we remark that the backgrounds occurred in the subsidiary multisingular points representing pure Ising and XY critical behaviour; thus in the total magnetic susceptibility $\chi = \frac{1}{3}\chi_\parallel + \frac{2}{3}\chi_\perp$, which is the best function to consider at the Heisenberg multisingular point, one sees that in a region of Ising-like behaviour, where only $\chi_\parallel$ diverges, the term $\frac{2}{3}\chi_\perp$ contributes a finite but relatively large and unavoidable background.)

It should perhaps be mentioned at this point (see also Fisher 1977, Fisher and Kerr 1977) that the partial differential equation (1.7) represents, from one viewpoint, a very natural generalisation to functions of two variables of the one-variable D log Padé technique. Thus, as observed by Gammel (1973) and Gaunt and, independently, by Guttmann and Joyce (1972), the D log approximant $[L/M]_{D\log f}$ may be regarded as providing for the approximation of $f(x)$ by the solution $F_{L;M}(x)$ of an ordinary linear homogeneous differential equation of the form (1.7), but with $R_N \equiv 0$ and with P_L and Q_M polynomials in the single variable x. Gammel and, in effect, Guttmann and Joyce called attention to the possibility of using more general differential equations to provide approximants to $f(x)$. Indeed, it is in this direction that the problem we have posed may be answered as we now show. (See also Baker and Moussa (1978) and Baker and Hunter (1978).)

2. Inhomogeneous differential approximants

To approach the problem of approximating effectively a function $f(x)$ of the form (1.4) let us calculate the derivative $f'(x) = \mathrm{d}f/\mathrm{d}x$ and eliminate the factor $(1-x/x_c)^\gamma$. One then sees that $f(x)$ is equal to the solution of the differential equation

$$U(x) + P(x)F(x) = Q(x)\,(\mathrm{d}F/\mathrm{d}x), \tag{2.1}$$

which satisfies the initial condition $F(0) = f(0) = f_0$, provided the coefficient functions are given by

$$\begin{aligned} U(x) &= (x_c - x)A(x)B'(x) - [\gamma A(x) + (x_c - x)A'(x)]B(x), \\ P(x) &= \gamma A(x) + (x_c - x)A'(x), \qquad Q(x) = (x_c - x)A(x). \end{aligned} \tag{2.2}$$

To ensure uniqueness we should also assume that $x = 0$ is a regular point of the equation, i.e. $Q(0) \neq 0$. Note furthermore that, if $A(x)$ and $B(x)$ are polynomials, then so are $U(x)$, $P(x)$ and $Q(x)$. If the background $B(x)$ vanishes, then so does $U(x)$; conversely, if $f(x)$ satisfies the homogeneous equation (with $U \equiv 0$), then for any added background term there is a corresponding $U(x)$ such that that inhomogeneous equation is satisfied by the new $f(x)$.

These considerations naturally suggest the definition of an *inhomogeneous differential approximant*, which may be denoted $F_{J/L;M}(x) = [J/L; M]_f$, as the solution of the equation

$$U_J(x) + P_L(x)F(x) = Q_M(x)\,(\mathrm{d}F/\mathrm{d}x), \tag{2.3}$$

with initial condition $F(0) = f(0) = f_0$, where the polynomial coefficient functions $U_J(x) = \Sigma_{j=0}^{J} u_j x^j$, etc are chosen so that the power series expansion of the solution $F(x)$ agrees with (1.1) as far as possible and, in particular, at least to order $x^{J+L+M+2}$; in addition, the normalisation condition

$$P_L(0) = p_0 = 1, \tag{2.4}$$

or, better in some circumstances, $Q_M(0) = q_0 = 1$, is imposed.

Such first-order linear inhomogeneous approximants were proposed explicitly by Gammel (1973) and are implicit in the ideas of Guttmann and Joyce (1972), although they studied (via a 'recursion relation' approach) only homogeneous cases. More recently Rehr *et al* (1979) also mention the inhomogeneous case explicitly but do not explore its properties. However, after completing the work reported here, we learned that Baker and Hunter (1979) have independently studied the $[J/L; M]_f$ approximants as defined above, although our viewpoints and applications have been complementary. The notation introduced above agrees with Baker and Hunter; however, they proposed the terminology 'integral approximants', since $f(x)$ is approximated by an integral curve of a differential equation. Note that, if Q_M is chosen to vanish identically, which may be denoted by the 'empty set' symbol $\varnothing$, one has $[J/L; \varnothing]_f \equiv [J/L]_f$, i.e. the approximant reduces to an ordinary direct Padé approximant. Conversely, if U_J is chosen to vanish, one has $[\varnothing/L; M]_f \equiv [L/M]_{D \log f}$, so that the standard D log Padé approximant is recaptured. Thus the inhomogeneous approximants interpolate in a rather natural way.

The proposed notation extends naturally as $[J/L; M; N]$, etc to cover cases in which a second-order derivative term $R_N(x)(\mathrm{d}^2F/\mathrm{d}x^2)$, etc is included, as discussed specifically by Guttmann and Joyce (1972, also Rehr *et al* 1979) in order to allow for possible confluent singularities.

In addition, we similarly propose *inhomogeneous partial differential approximants*, denoted $F_{\boldsymbol{J}/\boldsymbol{L};\boldsymbol{M},\boldsymbol{N}}(x, y) = [\boldsymbol{J}/\boldsymbol{L}; \boldsymbol{M}, \boldsymbol{N}]_f$, which, by analogy with (1.7), are solutions of

$$U_{\boldsymbol{J}}(x, y) + P_{\boldsymbol{L}}(x, y)F = Q_{\boldsymbol{M}}(x, y)\,(\partial F/\partial x) + R_{\boldsymbol{N}}(x, y)\,(\partial F/\partial y), \tag{2.5}$$

which satisfy appropriate boundary conditions and whose series expansions match that in (1.5) on powers $x^k y^{k'}$ with (k, k') in a maximal label set $\boldsymbol{K}$. Again, a normalisation condition $P_{\boldsymbol{L}}(0, 0) = p_{00} = 1$ will normally be appropriate; likewise, the polynomial coefficients $u_{jj'}$, $p_{ll'}$, $q_{mm'}$ and $r_{nn'}$ may be computed by solving linear algebraic equations.

We note specifically that a function $f(x, y)$ of the form

$$f(x, y) = A(x, y)\Delta\tilde{x}^{-\gamma} Z\left(\frac{g(x, y)\Delta\tilde{y}}{(h(x, y)\Delta\tilde{x})^{\phi}}\right) + B(x, y) \tag{2.6}$$

satisfies (2.5) for general $Z(z)$ if A, B, g and h are polynomials and

$$\begin{aligned} Q_{\boldsymbol{M}} &= A\Delta\tilde{y}[\phi gh/e_2 - (\phi gh_y - g_y h)\Delta\tilde{x}] + Agh\Delta\tilde{x}, \\ R_{\boldsymbol{N}} &= A\Delta\tilde{y}[\phi gh + (\phi gh_x - g_x h)\Delta\tilde{x}] + Aghe_1\Delta\tilde{x}, \end{aligned} \tag{2.7}$$

together with similar but longer explicit polynomial expressions for $U_{\boldsymbol{J}}$ and $P_{\boldsymbol{L}}$, which are not worth reproducing. (Recall that $\Delta\tilde{x}$ and $\Delta\tilde{y}$ are defined in (1.6); a subscript x or y denotes a corresponding partial derivative.) Evidently, an inhomogeneous partial differential approximant can represent effectively multisingular scaling behaviour with an added background. The generalisation to more variables is obvious.

From our present viewpoint the most important aspect of an inhomogeneous differential approximant is its behaviour in the vicinity of an anticipated singular point. Consider the single-variable approximants defined by (2.3): one expects to find a simple zero of the derivative coefficient $Q_M(x)$ at $x = x_0$. Then x_0 represents an estimate for the singular point x_c. In the neighbourhood of x_0 one may construct the expansions

$$U_J(x)=U_0+U_0'(x-x_0)+\mathrm{O}[(x-x_0)^2], \tag{2.8}$$

$$P_L(x)=P_0+P_0'(x-x_0)+\mathrm{O}[(x-x_0)^2], \tag{2.9}$$

$$Q_M(x)=Q_0'(x-x_0)+\tfrac{1}{2}Q_0''(x-x_0)^2+\mathrm{O}[(x-x_0)^3]. \tag{2.10}$$

Then it is not hard to see (Baker and Hunter (1979) give some explicit details) that, in general, the representation (1.4) holds, with x_0 replacing x_c, and with $A(x)$ and $B(x)$ analytic in the neighbourhood of x_0, while the exponent γ is given by

$$\gamma=-P_0/Q_0'. \tag{2.11}$$

This is essentially the same result as for standard D log Padé approximants. If γ should turn out to be an integer, the simple power law representation (1.4) may fail and special considerations are needed, as discussed by Baker and Hunter (1979).

Baker and Hunter present integral expressions for $A(x)$ and $B(x)$ in terms of U_J, P_L and Q_M; these may be found by solving (2.3) explicitly with the aid of an integrating factor. In the vicinity of x_0, however, we may express the background more simply as

$$B(x)=B_0+B_0'(x-x_0)+\ldots, \tag{2.12}$$

with

$$B_0=-U_0/P_0, \qquad B_0'=(P_0'U_0-P_0U_0')/P_0(P_0-Q_0'). \tag{2.13}$$

These results may be found easily by substituting power series expansions about x_0 into (2.3); similar but lengthier expressions are found for B_0'', etc. (In fact, the Baker–Hunter expression for $B(x)$ is not easy to deal with in the vicinity of x_0.)

The amplitude factor may be written

$$A(x)=A_0[1+a_1(x-x_0)+\ldots], \tag{2.14}$$

and substitution then yields (γ being non-integral)

$$a_1=(P_0'+\tfrac{1}{2}\gamma Q_0'')/Q_0', \tag{2.15}$$

and similar expressions may be found for a_2, etc. However, A_0 is necessarily given by an integral expression. Baker and Hunter give one formula, but it involves a singular integrand at the end of the range (which they handle by a special finite-difference approximation). An alternative expression which reduces the singularity by subtraction is

$$A_0=\frac{f_0}{Y_0}-B_0+\int_0^{x_0}\left(\gamma B_0-\frac{U_J(w)Y(w)}{V_{M-1}(w)Y_0}\right)\left(1-\frac{w}{x_0}\right)^{\gamma-1}\frac{\mathrm{d}w}{x_0}, \tag{2.16}$$

where γ and B_0 are defined by (2.11) and (2.13), while

$$Y(x)=\exp\left(-\int_0^x\frac{W_{L-1}(w)}{V_{M-1}(w)}\mathrm{d}w\right), \qquad Y_0=Y(x_0), \tag{2.17}$$

in which the polynomials V_{M-1} and W_{L-1} are defined by

$$V_{M-1}(x)=Q_M(x)/(x-x_0), \qquad W_{L-1}(x)=(P_L(x)+\gamma V_{M-1}(x))/(x-x_0). \tag{2.18}$$

Because of the subtraction, the integrand in (2.16) varies only as $(1-w/x_0)^\gamma\to 0$ as $w\to x_0$; nonetheless, if γ is small, some care may be needed to avoid loss of accuracy in evaluating the integral in this region.

Clearly, the evaluation of A_0 for a particular $[J/L; M]$ approximant is somewhat cumbersome. In practice it may well be easier and just as effective to estimate A_0, and thence the full function $f(x)$, by choosing a suitable background polynomial $\tilde{B}(x)$, which reproduces the 'best estimates' for B_0, B_0', etc, and forming direct Padé approximants to the amplitude function

$$\tilde{A}(x) = (f(x) - \tilde{B}(x))(1 - x/x_0)^{\gamma}, \tag{2.19}$$

in which x_0 and γ are, likewise, best estimates.

The analysis of the two-variable partial differential approximant defined by (2.5) in the multisingular region follows a similar route. As in the homogeneous case (Fisher and Kerr 1977), an estimate for the multisingular point (x_c, y_c) is provided by a common zero (x_0, y_0) of $Q_{\boldsymbol{M}}(x, y)$ and $R_{\boldsymbol{N}}(x, y)$. The exponents γ and ϕ and the scaling axis slopes e_1 and e_2 may then be estimated in terms of $P_0 = P_{\boldsymbol{L}}(x_0, y_0)$ and the gradients $(\partial Q_M/\partial x)_0$, etc by the same expressions as in the homogeneous case. Finally the background contribution at the multisingular point is estimated by

$$B_0 = -U_0/P_0, \qquad \text{with} \quad U_0 = U_{\boldsymbol{J}}(x_0, y_0), \tag{2.20}$$

in precise analogy to (2.13).

It is appropriate to mention at this point that Baker and Hunter (1979) have established a number of general properties of the $[J/L; M]$ and higher-order, single-variable inhomogeneous approximants. In particular, they show that the $[L/L; L+2]$ approximant is invariant under the Euler transformation $x = aw/(1+bw)$, as are direct, diagonal or $[L/L]$ Padé approximants (e.g. Baker 1975). Incidentally, they also prove that higher-order differential approximants cannot exhibit Euler invariance.

As in the construction of an ordinary Padé approximant, the linear equations for the polynomial coefficients defining an approximant $[J/L; M]$ or $[\boldsymbol{J}/\boldsymbol{L}; \boldsymbol{M}, \boldsymbol{N}]$ may either (i) be inconsistent, or (ii) have vanishing determinants. In the former case no approximant of the order sought exists; in the latter case one expects, nonetheless, to obtain a *unique* approximant, as happens for ordinary $[L/M]$ approximants where a common factor merely cancels from numerator and denominator. We have not succeeded in proving uniqueness, but in the Appendix we present a simple soluble example that demonstrates that uniqueness may be produced in a rather subtle way!

Finally, it should be pointed out that, as in the case of ordinary Padé approximants, one may impose at essentially no cost in computational difficulty a specified zero in one or more of the polynomial coefficients. In particular, if the singular point x_c is known (either exactly or with reasonable confidence), its value may be used to provide the additional coefficient equation

$$Q_M(x_c) = \sum_{m=0}^{M} x_c^m q_m = 0. \tag{2.21}$$

Then one fewer expansion coefficient f_i is needed to generate the corresponding 'biased' $[J/L; M]$ approximants; conversely, for given $\{f_i\}$ one may examine approximants of higher order.

In some cases one might also wish to specify the value of the exponent γ. The result (2.11) then yields the additional coefficient equation

$$P_L(x_c) + \gamma Q_M'(x_c) = \sum_{l=0}^{L} x_c^l p_l + \sum_{m=1}^{M} m\gamma x_c^{m-1} q_m = 0, \tag{2.22}$$

which can be accommodated with equal ease. In other circumstances arising in practice (e.g. Fisher 1974, Baker 1975), it may be desirable to fix γ but leave x_c free. This is more difficult, since imposition of (2.21) and (2.22), with x_c a variable, leads to a nonlinear problem which, at very least, impedes computation. A more desperate stratagem would be to take $M = L+1$ and impose $P_L(x) = -\gamma Q'_{L+1}(x)$ as a polynomial identity (the prime, as above, denoting a derivative): this leaves linear equations for the coefficients but, since it imposes the same exponent γ on all branch points of the approximant, is unlikely to lead to useful results in any but the most special circumstances.

Lastly, note from (2.13) that, given a value for x_c, one may fix the background terms B_0, B'_0, etc, in addition, or as an alternative, to specifying γ, and still retain linear equations for the coefficients.

3. Some applications

We now discuss some applications of the inhomogeneous differential approximants $[J/L; M]$ which illustrate their power and reveal some of their limitations. Baker and Hunter (1979) have tested the approximants on a number of specially constructed model test functions exhibiting various explicitly known types of singularity. Our computations have been complementary in that we have studied examples arising in practice where the exact behaviour is not known but where other methods of series analysis have given information which may be regarded as reasonably reliable.

3.1. *Ising model spin-$\frac{1}{2}$ high-temperature susceptibility expansions*

As a first group of examples we have examined the series expansions for the susceptibility $\chi(\equiv f(x))$ of spin-$\frac{1}{2}$ Ising models on three-dimensional lattices (Sykes *et al* 1972a) in powers of $x \equiv v = \tanh(J_1/k_B T)$, where J_1 is the nearest-neighbour exchange coupling and T is the temperature. These series are rather well-behaved, and on the basis of ratio analysis (e.g. Fisher 1974) the critical-point values x_c are known to a precision of about 1 part in 10^4 or better; it is also believed that $\gamma = 1{\cdot}250$, with an uncertainty of, say, $\pm 0{\cdot}004$ for all the lattices (Sykes *et al* 1972a). These ratio estimates are supported by standard D log Padé analysis. As an initial test, then, we studied the available series for the diamond, SC, BCC and FCC lattices (Gaunt and Sykes 1973, Sykes *et al* 1972a) with $J = 0, 1, \ldots, 5$ to see if any significant changes in the x_c and γ estimates would be caused by allowance for a background term. Here, and in most of the following work, we examine, in the interests of economy, only inhomogeneous approximants that are 'near diagonal' in the sense that $M = L, L\pm 1$.

A feel for the general character of the results can be gained from figure 1 which represents a plot of the exponent (γ) and background (B_0) estimates against the critical-point estimates, for most of the $[J/L; M]$ approximants which use terms from order v^{11} to v^{15} in the BCC susceptibility series; included are the standard D log Padé approximants $[\varnothing/5; 5]$ and $[\varnothing/7; 7]$, denoted by full circles, and the proper inhomogeneous approximants $[5/2; 2]$ and $[5/4; 4]$. A number of approximants are missing from the plot since they are seriously 'defective', as often observed in ordinary Padé approximation studies, in that they have spurious singularities on (or near) the real x axis closer to the origin than x_c, which leads to poor estimates. For the susceptibility series such defects seem somewhat more abundant for the larger values of J. In other cases quite distinct approximants yield graphically identical estimates.

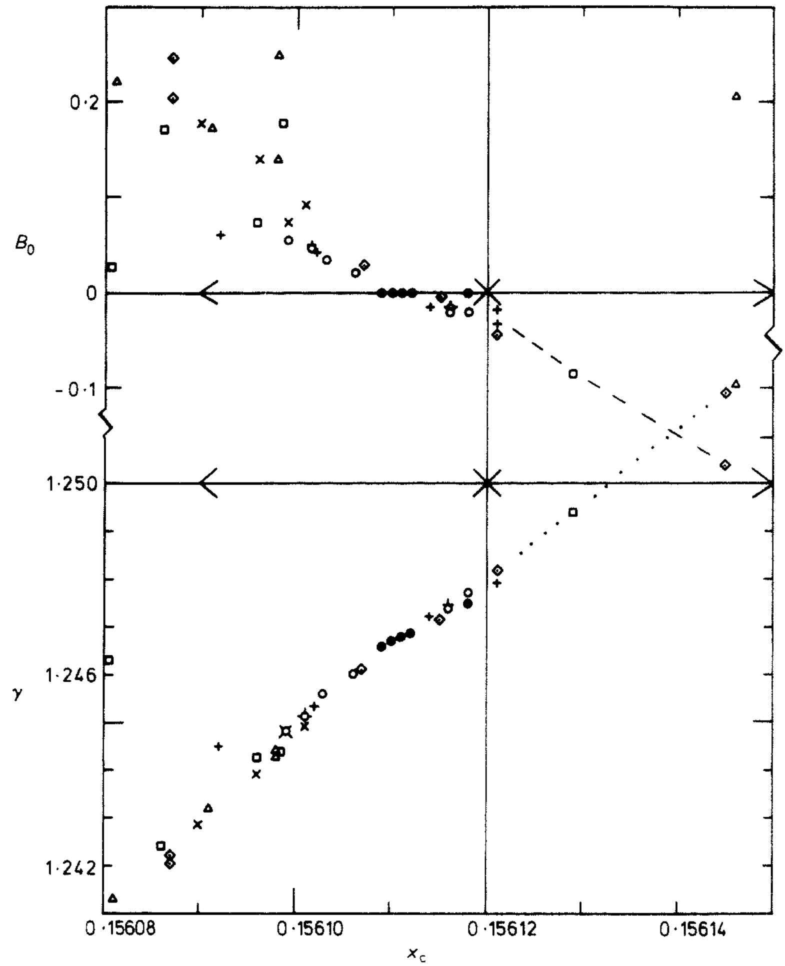

Figure 1. Estimates for the critical point x_c, exponent γ and background B_0 for the spin-$\frac{1}{2}$ Ising model BCC susceptibility series obtained from $[J/L; M]$ approximants for the values of J indicated by the various symbols: ●, $J \equiv \varnothing$; ○, $J = 0$; +, 1; ×, 2; △, 3; □, 4; ◇, 5. (The broken and dotted lines serve merely to link estimates for B_0 and γ respectively.) The large crosses and arrow heads indicate the ratio estimates and their limits.

Note, firstly, that the x_c scale in figure 1 is much magnified: it hardly exceeds the range of the ratio estimates, namely $x_c = 0{\cdot}15612 \pm 3$ (Sykes *et al* 1972a). The accepted ratio estimates and their limits are shown by large crosses and arrow heads. Evidently, the estimates for $J = 0, 1, 2, \ldots$ are rather more disperse than for $J \equiv \varnothing$; but for the most part they are encompassed within the ratio uncertainty limits (although one might, even for $J \equiv \varnothing$, prefer a central estimate for γ closer to 1·246 or 1·247). Secondly, it is clear that the marked correlation between the γ and x_c estimates, seen in Padé studies, is reproduced here. A similar correlation, but with rather more scatter, occurs in the (B_0, x_c) estimates. The background estimates are numerically very small, but one might well take $B_0 \simeq -0{\cdot}02 \pm 7$ as a best estimate for the BCC lattice. However, since $\gamma > 1$ (and $A_0 \simeq 1$), this will make negligible numerical difference in overall approximants to $\chi(v)$. For the FCC, SC and diamond lattices small negative backgrounds of comparable magnitude are also suggested. In summary, allowance for a background term in well-behaved series such as these leads to somewhat more disperse estimates for γ and x_c, but does not appear to degrade the overall precision.

3.2. *Transformation of initial coefficients*

In order to check the ability of the inhomogeneous approximants to handle changes in the first few terms of a series expansion, we have examined approximants to the modified series

$$\bar{\chi}_{\mathrm{diam}}(v)=\chi_{\mathrm{diam}}+2-9v=3-5v+12v^2+\ldots, \tag{3.1}$$

$$\bar{\chi}_{\mathrm{SC}}(v)=\chi_{\mathrm{SC}}-1+5v=0+11v+30v^2+\ldots, \tag{3.2}$$

$$\bar{\chi}_{\mathrm{BCC}}(v)=\chi_{\mathrm{BCC}}+2+7v=3+15v+56v^2+\ldots, \tag{3.3}$$

for $J\equiv\varnothing$ and $J=0, 1, 2$. As anticipated, the accuracy of the lower-order D log Padé approximants is seriously disturbed by these changes. However, for the SC lattice, where the expected change in background in the critical region is only about 0·09, the terms of order v^{16} and v^{17} still yield reasonably good estimates for x_c and γ.

For the diamond lattice the $J=\varnothing$ and $J=1$ approximants yield x_c to a precision reduced by a factor of about 10 and suggest exponents of around 1·20 and 1·16 with uncertainties of ±0·03. However, approximants with $J=1$ and 2, which can faithfully represent the added terms, lead to considerably improved estimates for x_c (although not so precise or so consistent as for the original series). Likewise, the exponent estimates now lie in the vicinity 1·23 to 1·24. This is a significant improvement, even though the quality of the estimates remains somewhat degraded relative to the original series.

The simple D log Padé estimates for the modified BCC series yield critical points with a precision of only 3 in 10^3 (compared with 2 in 10^4 from ratio estimates) and suggest the high values $\gamma=1{\cdot}28$ to 1·35. In this case good accuracy is restored by going to any of the inhomogeneous approximants with $J=0$, 1 or 2. The background now expected for the modified series is $\bar{B}_0\simeq 2+7v_c-0{\cdot}02\simeq 3{\cdot}07$. As is clear from table 1, all the higher-order inhomogeneous approximants are successful in generating this relatively large value to within a precision of about ±0·2.

3.3. *Specific heat expansions for the spin-$\frac{1}{2}$ Ising model*

The specific heats $C(v)$ of three-dimensional Ising models at high temperature diverge only weakly, with exponent $\gamma\equiv\alpha\simeq\frac{1}{8}$, and ratio analysis indicates they have significant

Table 1. Estimates of the critical-point background term $\bar{B}_0$ for the BCC spin-$\frac{1}{2}$ Ising susceptibility expansion modified as in equation (3.3). The expected value is $\bar{B}_0\simeq 3{\cdot}07$.

[0/5; 6] 3·202	[0/6; 5] 3·002	[0/6; 6] 3·203	[0/7; 5] 2·982	[0/6; 7] 3·138	[0/7; 6] 3·148
[1/5; 5] 3·299	[1/5; 6] 3·200	[1/6; 5] 3·359	[1/6; 6] 3·128	[1/5; 7] 3·128	[1/7; 5] 3·169
[2/4; 5] 3·304	[2/5; 4] 3·308	[2/5; 5] 3·303	[2/4; 6] 3·302	[2/5; 6] 3·075	[2/6; 5] 3·228

negative backgrounds in the critical region (Sykes *et al* 1972b). The D log Padé approach is very poor in these circumstances, even for a long series, as is clear from the first column of table 2. On the other hand, table 2 reveals that inhomogeneous approximants give a far better account of the singular behaviour once a reasonably long series is available. (Note that on standard Ising model conventions the terms f_0 and $f_1 v$ vanish identically in the specific heat series; we have analysed both the series $C(v)/v^2$ and $C(v)$, but always quote the values of B_0 which refer to $C(v)$.) The estimates for B_0 corresponding to the data in table 2 (and other inhomogeneous approximants not explicitly listed) suggest values in the range $-1\cdot0$ to $-1\cdot4$.

Table 2. Estimates for critical point v_c and exponent α for the high-temperature specific heat expansion of the FCC Ising lattice obtained from selected approximants $[J/L; M]$. Accepted estimates are $v_c \simeq 0\cdot10174$ and $\alpha \simeq 0\cdot125$.

$[J/L;M]$	v_c	α	$[J/L;M]$	v_c	α	$[J/L;M]$	v_c	α
[∅/2; 2]	0·12024	0·973	[0/2; 1]	0·11309	0·670	[1/1; 1]	0·11174	0·405
[∅/3; 3]	0·12425	1·012	[0/3; 3]	0·10204	0·146	[1/2; 2]	0·12310	0·961
[∅/4; 4]	0·10539	0·594	[0/4; 4]	0·10260	0·264	[1/3; 2]	0·10793	0·811
[∅/5; 5]	0·10434	0·550	[0/5; 5]	0·10185	0·135	[1/4; 4]	0·10224	0·206
[∅/6; 6]	0·10218	0·393	[0/5; 6]	0·10178	0·121	[1/5; 5]	0·10176	0·122

It is generally agreed that the most precise estimates for the critical points of Ising models are obtained from analysis of the high-temperature susceptibility series. On this basis we may accept, in particular, $v_c = 0\cdot15612 \pm 3$ for the BCC lattice (Sykes, Gaunt *et al* 1972) and use this to impose the value of $x_c \equiv v_c$ on the inhomogeneous approximants, as explained in (2.21) above. The BCC lattice is appropriate as a test case, since $C(v)$ has an expansion in even powers and only eight non-zero coefficients are known. We have performed the corresponding calculations for the SC and FCC lattices with quite similar results. Figure 2 shows how the exponent estimates for fixed v_c behave as a function of the total number of coefficients in the series which are used. Evidently the standard D log Padé approximants still do very badly. With $J = 0$ the inhomogeneous approximants indicate a far more rapid approach to a limit. For $J \geq 1$ even low-order approximants suggest exponent values in the range $0\cdot11$ to $0\cdot14$, and the overall picture clearly confirms the ratio estimate $\alpha \simeq 0\cdot125$. The SC data indicate a similar value, although the FCC data tend to indicate a somewhat lower value of about $0\cdot115$. Within the uncertainty limits, however, the exponent seems to be universal for all the three-dimensional lattices, as concluded in the ratio analysis (Sykes *et al* 1972b).

We have also checked the sensitivity of the exponent estimates to the choice of v_c imposed. In the BCC lattice a change from $v_c = 0\cdot15612$ to $v_c = 0\cdot15610$ decreased the estimates for α by about $0\cdot0015$; this is quite in line with the sensitivity observed in normal D log Padé analysis. The corresponding changes in the estimates of B_0 were of order $-0\cdot01$ to $-0\cdot03$, as might reasonably have been anticipated. As regards the actual value of the background term, figure 3 shows, for most of the approximants appearing in figure 2, the estimates for B_0 associated with a particular exponent estimate. A strong and remarkably sharp correlation is observed. The ratio estimates $\alpha = 0\cdot125$, $B_0 = -1\cdot248$ (Sykes *et al* 1972b) are shown by the large cross and arrow heads: it is surprising, given α, how closely the ratio estimate for B_0 coincides with that which would be drawn from the evidence of the inhomogeneous approximants. The

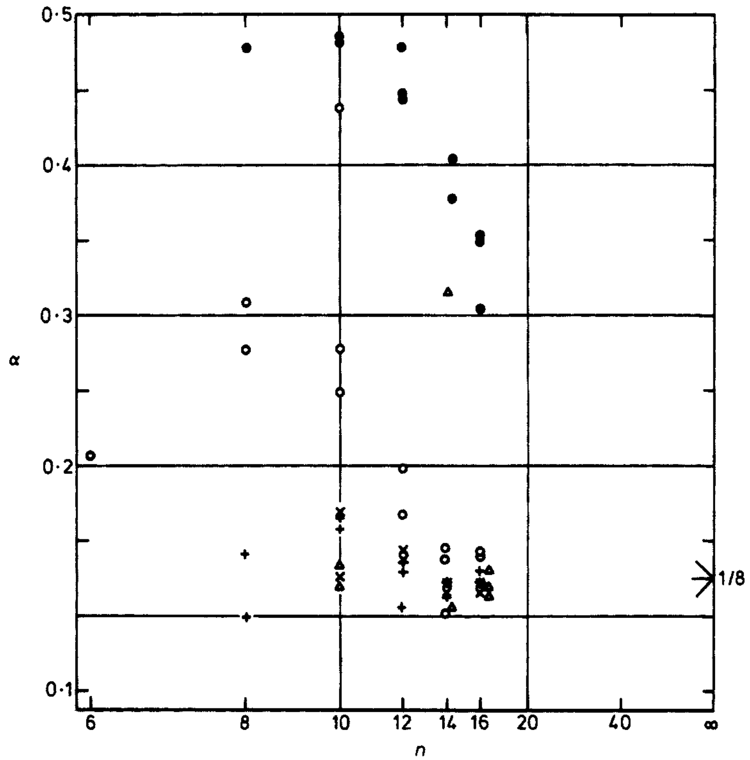

Figure 2. Estimates for the specific heat exponent α for the spin-$\frac{1}{2}$ Ising BCC model obtained from $[J/L; M]$ approximants with imposed critical point $v_c = 0{\cdot}15612$ for various values of J as a function of n, the power of v of the highest-order coefficient utilised: ●, $J \equiv \varnothing$; ○, $J = 0$; +, 1; ×, 2; △, 3. The preferred ratio estimate $\alpha = \frac{1}{8}$ is indicated on the right.

same coincidence is found for the FCC and SC lattices and strengthens one's confidence in the $[J/L; M]$ analysis.

3.4. *Antiferromagnetic spin-$\frac{1}{2}$ Ising susceptibilities*

Whereas the susceptibility of an Ising ferromagnet on a BCC or SC lattice exhibits a strong singularity of the form (1.4) with an exponent $\gamma \simeq 1{\cdot}25$, the corresponding antiferromagnet (obtained by changing the sign of the nearest-neighbour coupling energy J_1) is expected to display only the comparatively mild, non-divergent singular behaviour

$$\chi(v) \approx \chi_c + A_0(1 + v/v_c)^{-\gamma_0} + \ldots, \tag{3.4}$$

as $v \to -v_c$, with, in fact, $-\gamma_0 = 1 - \alpha \simeq 0{\cdot}88$ (see e.g. Sykes *et al* 1972a); in other words, the exponent γ is strongly negative, and the original background term B_0 thus becomes the dominant critical contribution χ_c. It is quite evident that direct or D log Padé approximants can give almost no significant information about such weak critical behaviour. Furthermore, since the signs of the appropriate series expansion coefficients now oscillate, the standard ratio analysis techniques are also not applicable in any straightforward way. Nonetheless, one may attempt to analyse the situation with the

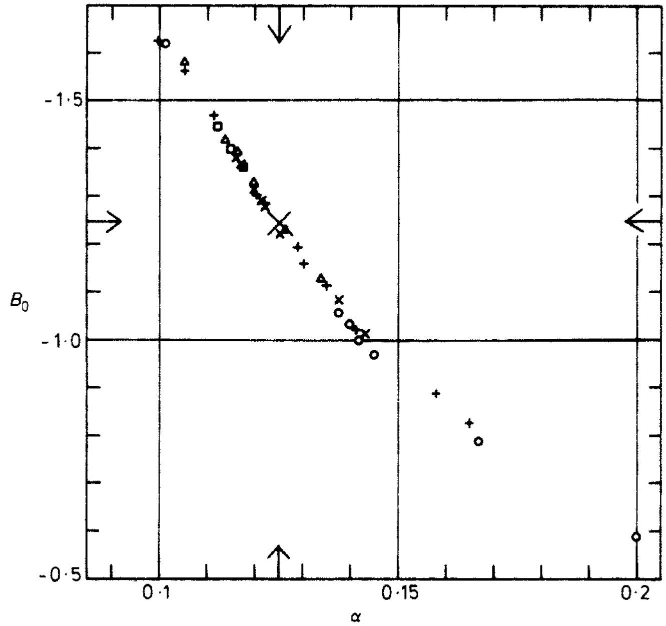

Figure 3. Variation of background estimates with exponent estimates using $[J/L; M]$ approximants with imposed critical point as in figure 2. The symbols denoting the values of J are the same as in figures 1 and 2; the large cross and arrow heads denote the ratio estimates.

aid of inhomogeneous approximants. Indeed, it suffices merely to examine the $[J/L; M]$ approximants previously calculated for the Ising ferromagnetic susceptibility expansions, at negative, real values of the variable $x \equiv v = \tanh(J_1/k_B T)$.

Now one knows on theoretical grounds that the antiferromagnetic singularity (on the SC and BCC lattices) must occur at $v_c^- = -v_c$, as implied in (3.4). Thus, as illustrated in the analysis of the specific heats just described, optimal estimates for $-\gamma_0$ and for $B_0 \equiv \chi_c$ should be obtained by imposing this value on the approximants. However, in order to test the ability of the $[J/L; M]$ approximants to detect such weak singularities, we report only on the results for 'unbiased' or 'free' approximants which themselves yield indications of the position of the singularity.

The results are, in fact, quite encouraging: thus for the SC lattice we find that the higher-order approximants for $J = 1, 2, 3, 4$ and 5 rather consistently indicate a singular point in the region $v_c^- \simeq -v_c(1 \pm \epsilon)$, with $\epsilon \simeq 0{\cdot}013$. Furthermore, as in figure 1, there is a strong monotonic correlation between the estimates for v_c^- and for the corresponding exponent estimates, which range from $-\gamma_0 \simeq 0{\cdot}6$ to $1{\cdot}1$, and with the background estimates B_0, which vary only over the comparatively small range from $0{\cdot}325$ to $0{\cdot}350$. However, if the preferred critical-point estimate $v_c^- = -v_c \simeq 0{\cdot}21817$ is adopted, one would conclude that $-\gamma_0 = 0{\cdot}86 \pm 3$ and $\chi_c \equiv B_0 \simeq 0{\cdot}3392 \pm 8$. These values compare surprisingly well with the theoretically expected value $-\gamma_0 \equiv 1 - \alpha = 0{\cdot}875 \pm 15 \simeq \frac{7}{8}$ and with the estimate $\chi_c \simeq 0{\cdot}3394$ obtained by Sykes *et al* (1972a), who do, in fact, utilise both the assumptions $v_c^- = -v_c$ and $-\gamma \equiv 1 - \alpha = \frac{7}{8}$. Comparable results have been obtained for the antiferromagnetic behaviour of the BCC and diamond lattices.

We conclude, therefore, that the inhomogeneous approximants are capable of resolving rather weak, non-divergent singularities with reasonable reliability. In a practical case, however, having detected such a singularity, one would probably prefer to analyse primarily the derivative series expansion in which the singularity should appear more strongly. Nevertheless, the ability of the inhomogeneous approximants to provide an indication of a weak singularity is clearly a valuable feature.

3.5. *Susceptibilities of the spin-∞ Heisenberg, XY and Ising models*

Our current numerical understanding of thermodynamic bicritical points is largely based on analyses of the high-temperature series for the susceptibility of the spin-∞ anisotropic Heisenberg model which includes the spin-∞ XY and Ising models as special limits (see Pfeuty *et al* 1974). The available series are not very long and, although susceptible to ratio analysis, are not as smooth or as well-behaved as the spin-$\frac{1}{2}$ Ising expansions (Pfeuty *et al* 1974, Camp and van Dyke 1975). Accordingly, we felt it worthwhile to analyse the expansions for the SC, BCC and FCC lattices using the $[J/L; M]$ approximants.

Our findings can be expressed conveniently by describing the plots of γ and B_0 estimates against x_c estimates as in figure 1. As there, rather clear and consistent loci, $\gamma \simeq \Gamma(x_c)$ and $B_0 \simeq B(x_c)$, emerge. However, by contrast with the spin-$\frac{1}{2}$ data, the standard D log Padé estimates for γ are spread over a wide range: thus, taking the $S=\infty$ FCC Ising series as an exemplar, one finds γ values of from 1·18 to 1·24. Conversely, the corresponding approximants for $J=0$ and, even more so, those for $J \geqslant 1$ yield rather well-clustered estimates, mainly in the range $\gamma = 1{\cdot}215$ to $1{\cdot}235$. On the basis of these data alone, one would probably conclude $\gamma = 1{\cdot}225 \pm 7$. At the same time, a rather precise value of B_0, namely $-0{\cdot}13$, is indicated for the central value of γ (and of x_c); however, uncertainties in B_0 of $\pm 0{\cdot}05$ correlate with the range of uncertainty in γ (and x_c).

The estimate for γ found here, and similarly the estimates for the XY and Heisenberg $S=\infty$ models, agree closely with those obtained by ratio analyses (see e.g. Pfeuty *et al* 1974). In each case, however, a significant background term is found, in contrast to the $S=\frac{1}{2}$ susceptibility functions. On the other hand, the discrepancy between the Ising spin-$\frac{1}{2}$ estimate of $\gamma \simeq 1{\cdot}25$ and the Ising spin-∞ estimates of $\gamma \simeq 1{\cdot}22$ to 1·23 is not resolved by the use of inhomogeneous approximants. The hypothesis of critical-exponent universality suggests these values should be identical; however, the true reason for this difference (real or apparent as it may be) is not fully understood. Nevertheless, it has been suspected as being an artefact caused by the presence of *confluent* singularities. When $\gamma \geqslant 1$ such confluent singularities cannot be well approximated by inhomogeneous approximants, so it is not really surprising that their use sheds no special new light on this question. However, the data from the $[J/L; M]$ studies strongly indicate that an optimal representation of the spin-∞ susceptibilities should allow for a background contribution.

3.6. *The Yang–Lee edge singularity*

It has recently been observed (Baker and Moussa 1978, Fisher 1978) that the nature of the singularity at the edge of the Yang–Lee distribution of zeros in the complex magnetic field plane of an Ising ferromagnet can be understood in the high-temperature limit by studying the activity expansions of a gas of hard dimers on the corresponding lattice. The resulting series expansions for two- and three-dimensional lattices display considerable curvature in ratio analyses which make them difficult to extrapolate with confidence. The standard D log Padé techniques similarly give disperse and non-convergent results. It has been found, however, that rather consistent and apparently reliable estimates are given by $[J/L; M]$ approximants. Furthermore, the Bethe lattice series, for which the exact behaviour is known (Baker and Moussa 1978), prove very troublesome for the standard techniques, but are remarkably well represented by inhomogeneous approximants. The detailed results of this study will be reported elsewhere (Kurtze and Fisher, 1979).

3.7. Low-temperature Ising model series

Baker and Hunter (1979) have applied inhomogeneous differential approximants to re-examine the exponent of divergence, γ', of the low-temperature susceptibilities of three-dimensional Ising lattices. Standard D log Padé analysis tends to suggest $\gamma' \simeq 1{\cdot}30$, whereas the scaling hypothesis leads one to expect the same exponent as for the high-temperature expansions, namely $\gamma \simeq 1{\cdot}25$. The low-temperature expansions are notoriously difficult to analyse, in that there are strong, interfering singularities in the complex plane (the number depending on the lattice) which lie closer to the origin than the real, physical singularity. Nevertheless, with the aid of $[J/L; M]$ approximants, Baker and Hunter obtained quite convincing evidence that, when the series expansion is long enough relative to the number of interfering singularities, the BCC lattice being the best case, the low-temperature exponent γ' approaches the expected value $1{\cdot}25$.

We have elected to examine the corresponding series for the specific heats (Sykes *et al* 1965, 1973); in particular, we have studied the series for the FCC lattice which are long, but irregular:

$$\bar{C}(x) = 36x^2 + 726x^{11} - 936x^{12} + 1800x^{15} + 10\,752x^{16} - \dots \tag{3.5}$$

Here $\bar{C}$ is the reduced specific heat, while $x = \exp(-4J_1/k_BT)$ is the natural low-temperature variable; the last available term is $+47\,823\,031\,200x^{40}$. The expected exponent of divergence is small, namely $\alpha' \simeq 0{\cdot}125$. D log Padé approximants are quite disperse and suggest an exponent of $0{\cdot}25 \pm 0{\cdot}08$ and, correspondingly, a critical point about 0·7% higher than believed correct (on the basis of the high-temperature expansions). The inhomogeneous approximants for $J = 0$, 1, 2 and 3 improve the situation, but not dramatically. They are still quite disperse, suggesting $\alpha' \simeq 0{\cdot}21 \pm 0{\cdot}07$ and a critical point high by, perhaps, only 0·5%. If the value of x_c is imposed, the D log Padé approximants yield $\alpha' \simeq 0{\cdot}22 \pm 0{\cdot}02$; the inhomogeneous approximants are spread more widely, and correlated strongly with corresponding estimates for the background B_0. Plausible estimates might be $\alpha' \simeq 0{\cdot}19 \pm 0{\cdot}05$ and $B_0 \simeq -2{\cdot}0 \pm 2{\cdot}5$. The expected exponent value, $\alpha' \simeq 0{\cdot}125$, is not ruled out, but rather few approximants give estimates in that region. Nevertheless, if, as explained in § 2, both the value of x_c and of α were imposed, the inhomogeneous differential approximants should yield useful approximations to the specific heat functions themselves.

4. Summary

We feel the range of applications discussed above make it clear that the inhomogeneous differential approximants $[J/L; M]_f$ are useful and practicable tools for series analysis that should be used in most circumstances where the D log Padé technique alone might have been employed in the past. In many cases where there is a significant background contribution in the region of the expected branch-point singularity, the $[J/L; M]_f$ approximants will probably yield additional and more reliable information. In other cases they may merely confirm that the assumption of a negligible background, i.e. a purely factoring branch point, is reasonably well justified. Finally, the example of the low-temperature Ising specific heat series—probably among the most difficult series to analyse reliably—demonstrates that the inhomogeneous approximants are not a universal panacea. To expect otherwise, however, would be naive!

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Appendix. Examples illustrating uniqueness

Suppose the equations specifying the polynomials $U_J(x)$, $P_L(x)$ and $Q_M(x)$ in the $[J/L; M]$ approximant are indeterminate so there are many solutions parametrised by a number of arbitrary constants, say $c_1, c_2, \ldots, c_g$. One obvious mechanism by which the approximant itself could, nonetheless, be unique is *factorisation uniqueness*, in which

$$\begin{aligned} U_J(x) &= \bar{U}_{\bar{J}}(x) Z_I(x; \{c_k\}), \qquad P_L(x) = \bar{P}_{\bar{L}}(x) Z_I(x; \{c_k\}), \\ Q_M(x) &= \bar{Q}_{\bar{M}}(x) Z_I(x; \{c_k\}), \end{aligned} \tag{A1}$$

where the reduced polynomials $\bar{U}_{\bar{J}}(x)$, $\bar{P}_{\bar{L}}(x)$ and $\bar{Q}_{\bar{M}}(x)$ with $\bar{J} = J - I$, etc are independent of the $\{c_k\}$. Evidently, the arbitrary polynomial factor $Z_I(x; \{c_k\})$ cancels to leave a unique differential equation corresponding to the lower-order approximant $[\bar{J}/\bar{L}; \bar{M}]$. Provided $\bar{Q}_{\bar{M}}(0) \neq 0$, the condition $F(0) = f_0$ then yields a unique approximant. This is the mechanism of uniqueness in ordinary $[L/M]$ Padé approximants. A concrete example is provided by

$$f(x) = 2\,e^x - 1 = 1 + 2x + x^2 + \tfrac{1}{3}x^3 + \ldots. \tag{A2}$$

The five equations for the parameters u_0, u_1, $p_0 = 1$, p_1, q_0 and q_1 for the [1/1;1] approximant yield

$$U_1(x) = 1 + c_1 x, \qquad P_1(x) = 1 + c_1 x, \qquad Q_1(x) = 1 + c_1 x. \tag{A3}$$

Thus the factor $1 + c_1 x$ cancels from (2.3), and the [1/1;1] approximant reduces identically to the [0/0;0] approximant with $U_0 = P_0 = Q_0 = 1$; this actually reproduces (A2) exactly.

However, there is at least one other distinct mechanism which might be termed *integral uniqueness*. As an illustration, consider the [1/0; 1] approximant to

$$f(x) = e^{x^5} + 2x = 1 + 2x + x^5 + \ldots, \tag{A4}$$

for which, using the expansion to order x^4, one finds

$$U_1(x) = c_1 + c_2 x, \qquad P_0 \equiv 1, \qquad Q_1(x) = \tfrac{1}{2}(1 + c_1) + \tfrac{1}{2}(1 + c_2)x, \tag{A5}$$

so that there is certainly no common polynomial factor! The general solution of (2.3) may then be written

$$F(x)=1+2x+C_0(Q_1(x))^{2/(1+c_1)}, \tag{A6}$$

where C_0 is the arbitrary constant of integration. Provided $q_0=\frac{1}{2}(1+c_1)$ does not vanish, the only solution satisfying $F(0)=f_0=1$ is obtained for $C_0=0$. Thus the [1/0; 1] approximant is, in fact, unique and represents $f(x)$ correctly to $O(x^4)$ as it should.

References

Baker G A Jr 1975 *Essentials of Padé Approximants* (New York: Academic)
Baker G A Jr and Hunter D L 1979 *Phys. Rev.* B **19** 3808
Baker G A Jr and Moussa P 1978 *J. Appl. Phys.* **49** 1360
Camp W J and van Dyke J P 1975 *Phys. Rev.* B **11** 2579
Chisholm J S R 1973 *Math. Comput.* **27** 841
Chisholm J S R and Roberts D E 1976 *Proc. R. Soc.* A **351** 585
Fisher M E 1974 *Rocky Mtn J. Math.* **4** 181
—— 1977 *Statistical Mechanics and Statistical Mechanics in Theory and Application* ed U Landman (New York: Plenum) p 3
—— 1978 *Phys. Rev. Lett.* **40** 1610
Fisher M E and Kerr R M 1977 *Phys. Rev. Lett.* **39** 667
Gammel J L 1973 *Padé Approximants and their Applications* ed P R Graves-Morris (New York: Academic) p 3
Gaunt D S and Sykes M F 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1517
Guttmann A J and Joyce G S 1972 *J. Phys. A: Gen. Phys.* **5** L81
Kurtze D A and Fisher M E 1979 *Phys. Rev.* B (in press)
Pfeuty P, Jasnow D and Fisher M E 1974 *Phys. Rev.* B **10** 2088
Rehr J J, Joyce G S and Guttmann A J 1979 submitted to *J. Phys. A: Math. Gen.*
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 2
Sykes M F, Gaunt D S, Martin J L and Mattingly S R 1973 *J. Math. Phys.* **14** 1071
Sykes M F, Gaunt D S, Roberts P D and Wyles J A 1972a *J. Phys. A: Gen. Phys.* **5** 640
Sykes M F, Hunter D L, McKenzie D S and Heap B R 1972b *J. Phys. A: Gen. Phys.* **5** 667