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# Methods of series analysis. III. Integral approximant methods

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We discuss the approximation of functions by the solution of certain differential equations derived from their power-series coefficients. We call these approximations integral-curve approximants, or more simply integral approximants, and find that they include as special cases many of the currently used methods. We investigate their invariance and singularity properties, and test the power of the first-order ones on a series of known functions. These integral approximants do as well, and often better, than any of the now current (nonexact) methods of approximation. We have applied them to the low-temperature Ising-model susceptibility and find, for the first time by series methods, reasonably good evidence that the low-temperature critical index is equal to the high-temperature one, as expected from the scaling and renormalization-group approaches.

## I. INTRODUCTION AND SUMMARY

One quite successful approach to problems in critical phenomena, when exact solutions are unavailable, is to deduce the behavior of the system in the critical region from exact series expansions. The methods of analyzing series expansions have been reviewed by the authors[1] (hereinafter referred to as I) and by Gaunt and Guttmann.[2] In addition some new methods of analyzing series, especially appropriate for functions with specific singularity structure, were proposed by the authors[3] (II). The method of generalized approximants proposed in II works very well in some situations but has the disadvantage that systems of nonlinear equations must be solved to obtain the approximants. This computational problem has proven to be rather difficult and time consuming in the context of the problems encountered in critical phenomena, so much so that a diverse strategy of optimization[4] was employed to maximize the improvement in each iteration.

It is the purpose of this paper to examine the usefulenss and properties of approximants which are the solutions of differential equations. A solution of a differential equation being an integral curve of the equation, we suggest that these be called *integral-curve approximants* or, more simply, *integral approximants*.

Approximants of this type were first proposed by Guttmann and Joyce[5] and independently by Gammel[6] and Gaunt. The most general form they consider is approximants to $f(x)$ which satisfy

$$\sum_{\nu=0}^{K} Q_\nu(x) f^{(\nu)}(x) + R(x) = 0 \qquad (1.1)$$

to order $\kappa+1$ greater than the sum of the orders of the polynomial coefficients $Q_\nu(x), R(x)$, where $f^{(\nu)}$ means $d^\nu f/dx^\nu$. Guttmann and Joyce limit their applications to a special case of Eq. (1.1), i.e., to approximants which satisfy a second-order homogeneous equation $[K=2, R(x)\equiv 0]$. They call their method the *recurrence relation* method because they are able to develop a recurrence relation that enables them to obtain the coefficients of the polynomials.

Gammel has suggested the use of integral approximants derived from a first-order inhomogeneous form of Eq. (1.1), namely

$$Q_M(x) f'(x) + P_L(x) f(x) + R_N(x) = O(x^{L+M+N+2}) \quad . \qquad (1.2)$$

In this paper we will show that many of the other forms of series analysis are special cases of integral approximation. In particular, in Sec. II, we will show:

 

(A) Padé approximants and $D$ log Padé approximants are special cases.

(B) The ratio method and Neville Table extrapolation of ratio sequences are all special cases.

(C) The recurrence relation method is a special case (already shown).

(D) If a function satisfies the equation for quadratic Padé approximants,

$$P(x)f^2(x)+Q(x)f(x)+R(x)=0 \ , \tag{1.3}$$

then it satisfies Eq. (1.1).

(E) If a function is of the form of the generalized approximants introduced in II, then it satisfies Eq. (1.1).

In cases (D) and (E), above, the order $\kappa$ of Eq. (1.1) necessary to show equivalence tends to be quite high, and hence leads to no computational advantage.

We investigate the invariance of integral approximants under the homographic transformation

$$x=Aw/(1+Bw) \ . \tag{1.4}$$

In Sec. III we show that the most general integral approximant which possesses this invariance property has the form of Eq. (1.2), with $L=N=M-2$. Both $[N/N]$ diagonal Padé approximants and $[N,N,N]$ quadratic Padé approximants possess this invariance property, which is thought to greatly expand the region of convergence of sequences of diagonal (and even near-diagonal) sequences of the approximants. For a complete discussion of the invariance and convergence propeties of Padé approximants see Baker.[7]

In Sec. IV we investigate the nature of the first-order inhomogeneous integral approximants. We examine the behavior of various members of that class at the point of infinity. We also find the form of the solutions of Eq. (1.2) in the neighborhood of their singular points. Denoting the solutions of Eq. (1.2) as $[N/L;M]$, we show that near $x_i$

$$[N/L;M]\simeq A(x)\left(1-\frac{x}{x_i}\right)^{-\gamma_i}+B(x) \ , \tag{1.5}$$

where $A(x)$ and $B(x)$ are regular in that region, provided $\gamma_i$ is not a negative integer. We describe the procedure we use to calculate the remainder $B(x_i)$.

In Sec. V we study the application of the first-order approximants to the test functions introduced in I as benchmarks for the comparison of the effectiveness of different methods of series analysis. The test functions are shown in Table I. Because of the invariance property and variety of limiting behavior possessed by first-order integral approximants, we use these in our analysis, and compare their effectiveness with biased and unbiased forms of ratio, Padé, generalized approximant, and recurrence relation analysis. For some of the test functions we can show that second-order homogeneous integral approximants (recurrence relation method) represent the function exactly. Barring those cases we find that the first-order integral approximants are at least as good as, and often significantly better than, the other methods under consideration.

TABLE I. Test functions $A-K$ used to compare effectiveness of various methods of series analysis. Reproduced from I.

| | |
|---|---|
| $A.$ | $(1-x)^{-1.5}+e^{-x}$ |
| $B.$ | $(1-x)^{-1.5}(1+\frac{1}{2}x)^{1.5}+e^{-x}$ |
| $C.$ | $(1-x)^{-1.5}(1-\frac{1}{2}x)^{1.5}+e^{-x}$ |
| $D.$ | $(1-x)^{-1.5}+(1+\frac{1}{4}x^2)^{-1.25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1.25}$ |
| $E.$ | $(1-x)^{-1.5}(1+\frac{1}{2}x)^{1.5}+(1+\frac{1}{4}x^2)^{-1.25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1.25}$ |
| $F.$ | $(1-x)^{-1.5}(1-\frac{1}{2}x)^{1.5}+(1+\frac{1}{4}x^2)^{-1.25}+(1+\frac{15}{112}x-\frac{1}{4}x^2)^{-1.25}$ |
| $G.$ | $(1-x)^{-1.5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1.25}$ |
| $H.$ | $(1-x)^{-1.5}(1+\frac{1}{2}x)^{1.5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1.25}$ |
| $I.$ | $(1-x)^{-1.5}(1-\frac{1}{2}x)^{1.5}+\{2(1-x)(2-x)^6/[(2-x)^7-x^7]\}^{1.25}$ |
| $J.$ | $(1-x)^{-1.5}+(1+\frac{4}{5}x)^{-1.25}$ |
| $K.$ | $(1-x)^{-1.5}+(1+\frac{4}{5}x)^{-1.25}+e^{-x}$ |

Finally, in Sec. VI we analyze the low-temperature Ising susceptibility series using integral approximants. For each three-dimensional lattice we study, we have tabulated the biased estimates for $\gamma'$ according to the number of series coefficients used in obtaining each estimate. We observe a rather marked shift in the estimates toward $\gamma'\approx\gamma=1.25$. For each lattice this shift occurs for a particular number of terms, which seems to be smoothly dependent upon the number of singularities in the low-temperature series. In fact, it appears that for each additional singularity in the function six more series coefficients are required in order to see the estimates of $\gamma'$ shift from $\gamma'\gtrsim 1.30$ to $\gamma'\simeq 1.25$. The number of terms available relative to the number of singularities is most favorable for the bcc lattice, and hence the shift is most noticeable. However, there is evidence that such a shift has occurred for all 4 lattices studied. This shift has not been apparent in studies using other methods of analysis, and hence the bcc has often been regarded rather suspiciously since the $\gamma'$ estimates seemed anomalously low. We feel, however, that we have now obtained rather more convincing evidence that $\gamma'=\gamma$ than has previously been available from direct analysis of series expansions.

## II. RELATIONSHIP BETWEEN INTEGRAL APPROXIMANTS AND OTHER METHODS

The generalization to integral approximants is a logical one to make because it is possible to show that just about every method of analyzing series previously used is a special case of Eq. (1.1).

### A. Padé approximants

Padé approximants to the function under consideration may be formed directly

$$f(x)-\frac{\mathcal{P}_N(x)}{\mathcal{Q}_D(x)}=O(x^{N+D+1}) \;, \tag{2.1}$$

or more usually the derivative of the logarithm may be approximated by a Padé approximant

$$\frac{d}{dx}[[\ln f(x)]-\frac{\mathcal{P}_n(x)}{\mathcal{Q}_D(x)}=\frac{f'(x)}{f(x)}-\frac{\mathcal{P}_N(x)}{\mathcal{Q}_D(x)}$$
$$=O(x^{N+D+1}) \;. \tag{2.2}$$

Equation (2.1) is equivalent to Eq. (1.2), with $K=0$ and $R(x)\equiv\mathcal{P}_N(x)$, while Eq. (2.2) is equivalent to Eq. (1.2), with $K=1$ and $R(x)\equiv 0$. Not only are usual applications of Padé approximants a type of integral approximation, they are special cases of the first-order inhomogeneous case we consider in detail in the remainder of this paper.

### B. Ratio method and Neville extrapolation

That the ratio method and the Neville Table extrapolation of the ratios are special cases of integral approximants can be shown by considering the following equations

$$(1+a_0x)f+R_L(x)=O(x^{L+2}) \;,\quad \nu=0 \;, \tag{2.3}$$

$$(1+a_\nu x)\frac{d}{dx}\left[x\frac{d}{dx}\right]^{\nu-1}f+\sum_{j=0}^{\nu-1}a_j\left[x\frac{d}{dx}\right]^j f+R_L(x)$$
$$=O(x^{L+\nu+2}) \;,\quad \nu>0 \;. \tag{2.4}$$

These are special forms of Eq. (1.1) for a $\nu$th-order integral approximant.

Solving Eq. (2.3) for $-a_0$, we obtain the standard ratios

$$-a_0=\frac{\alpha_{L+1}}{\alpha_L}\equiv r_n \;, \tag{2.5}$$

where $\alpha_i$ are the coefficients in the series expansion for $f(x)$, and where $n=L+\nu+2-\delta_{\nu 0}$ is the customary subscript associated with the ratios or extrapolants—i.e., the order of the highest coefficient used in calculating that parameter. The expressions above and following are valid for all $L\geqslant -1$, where $R_{-1}(x)$ is defined to be identically zero.

If we solve Eq. (2.4) for $-a_\nu$, we obtain for $\nu=1$, the linear extrapolants $y_n$ of the ratios [which are estimates of $x_c^{-1}$; Eq. (2.5) of I].

$$-a_1=(L+3)r_{L+3}-(L+2)r_{L+2}=l_n^{(1)}=y_n \;; \tag{2.6}$$

for $\nu=2$, the 2nd-order Neville extrapolants are

$$-a_2=[(L+4)^2r_{L+4}-2(L+3)^2r_{L+3}$$
$$+(L+2)^2r_{L+2}]/2=l_n^{(2)} \;, \tag{2.7}$$

and for general $\nu$, the $\nu$th-order Neville extrapolants $l_n^{(\nu)}$, where $n=L+\nu+2-\delta_{\nu 0}$, is the order of the highest coefficient used in forming the extrapolant. The general solution for $-a_\nu$ can be shown to be

$$-a_\nu=(-1)^\nu\frac{1}{\nu!}\sum_{j=0}^{\nu}(-1)^j\binom{\nu}{j}$$
$$\times(L+j+2)^\nu r_{L+j+2} \;. \tag{2.8}$$

It is clear from Eqs. (2.5) to (2.7) above that [see also Eq. (2.26) of I]

$$-a_\nu=l_n^{(\nu)}=\frac{1}{\nu}[nl_n^{(\nu-1)}-(n-\nu)l_{n-1}^{(\nu-1)}] \tag{2.9}$$

for the first few values of $\nu$. The proof by induction that Eq. (2.9) is true generally follows in a straightforward way from Eq. (2.8).

Part of the usefulness of the ratio method lies in possibility of obtaining estimates (both biased and unbiased) for the critical exponent [Eqs. (2.6) and (2.7) of I]. If one solves the $\nu=1$ case of Eq. (2.4) for $a_0$, one obtains

$$a_0=(L+2)[(L+3)r_{L+3}-(L+2)r_{L+2}]-(L+3)r_{L+3}$$
$$=(n-1)[nr_n-(n-1)r_{n-1}]-nr_n$$
$$=(n-1)y_n-nr_n \;. \tag{2.10}$$

In Sec. III we show that the exponent associated with the singularity $x_c$ in $[N/L;M]$ is given by $P(x_c)/Q'(x_c)$. For $[L/0;1]$ this becomes

$$\frac{P(x_c)}{Q'(x_c)}=\frac{a_0}{a_1}=nr_ny_n^{-1}-n+1 \;, \tag{2.11}$$

which by Eq. (2.7) in I is $\gamma_n^{(u)}$, the unbiased exponent estimate obtained from the $n$th-order coefficient of the series expansion.

### C. Recurrence relation method

As stated in the introduction, Guttmann and Joyce[5] have shown that their recurrence relation method and its generalization to orders greater than two[8] yields an approximant which satisfies a homogeneous form of the differential equation (1.1) and is therefore a special case of integral approximation.

### D. Quadratic Padé approximants

Quadradic Padé approximants[9] to a function $f(x)$ satisfy

$$P_af^2+Q_bf+R_c=O(x^{a+b+c+2}) \;, \tag{2.12}$$

and therefore are the roots $\omega$ of

$$P_a\omega^2+Q_b\omega+R_c=0 \ , \tag{2.13}$$

where $a$, $b$, and $c$ are the degrees of the polynomials $P_a(x)$, $Q_b(x)$, and $R_c(x)$, respectively.

If a function exactly satisfies Eq. (2.13), then we can show that it also satisfies Eq. (1.2). First eliminate the linear term in Eq. (2.13) by substituting $u=\omega+Q/2P$, and Eq. (2.13) becomes

$$u^2=(Q^2/4P^2)-R/P \ . \tag{2.14}$$

Differentiating Eq. (2.14) and combining Eq. (2.14) with the derived equation, one obtains

$$(PQ^2-4P^2R)u'+(2P^2R'-PQQ'+P'Q^2-2PP'R)u=0 \ . \tag{2.15}$$

Substituting back for $\omega$, one gets

$$(PQ^2-4P^2R)\omega'+(2P^2R'-PQQ'+P'Q^2-2PP'R)\omega+(P'QR-2PQ'R+PQR')=0 \ . \tag{2.16}$$

It is obvious that the degree of the polynomial coefficients in the differential equation is greatly increased. Thus, the function $\omega$ can be written as a first-order integral approximant $[N/L;M]$, where

$$L=\max(a+2b,2a+c) \ ,$$
$$M=\max(2a+c-1,a+2b-1) \ , \tag{2.17}$$
$$N=a+b+c-1 \ .$$

### E. Generalized approximants

The pure generalized approximant form without Padé-type correction term as introduced in II is

$$F(x)\equiv F^{(0)}(x)=\sum_{i=1}^{N}A_i(1-y_ix)^{-\gamma_i}\equiv\sum_{i=1}^{N}X_i \ . \tag{2.18}$$

To show $F(x)$ satisfies Eq. (1.1), differentiate the function $F(x)$ $N$ times, writing the $j$th derivative as

$$F^{(j)}(x)=\sum_{i=1}^{N}\frac{B_{ji}}{(1-y_ix)^j}X_i \ , \tag{2.19}$$

where

$$B_{ji}=(\gamma_i)(\gamma_i-1)\cdots(\gamma_i-j+1)y_i^j \ , \quad j\geq 1$$
$$B_{0i}=1 \ .$$

We now have $N+1$ functions $F^{(0)},F^{(1)},\ldots,F^{(N)}$, which are linear in the $N$ variables $X_i$, and which, therefore, must be linearly dependent. Hence, the $(N+1)\times(N+1)$ determinant $D$ must vanish

$$D\equiv\begin{vmatrix} F^{(0)} & 1 & 1 & \cdots & 1 \\ F^{(1)} & \dfrac{B_{11}}{1-y_1x} & \dfrac{B_{12}}{1-y_2x} & \cdots & \dfrac{B_{1N}}{1-y_Nx} \\ \vdots & \vdots & \vdots & & \vdots \\ F^{(N)} & \dfrac{B_{N1}}{(1-y_1x)^N} & \dfrac{B_{N2}}{(1-y_2x)^N} & \cdots & \dfrac{B_{NN}}{(1-y_Nx)^N} \end{vmatrix}=0 \ . \tag{2.20}$$

Expanding $D$ about the first column, we find that the coefficient of $F^{(i)}$ has a polynomial of order $N(N+1)/2-i$ in $x$ in its denominator. If one factors $\prod_{i=1}^{N}(1-y_ix)^{-N}$ out of $D$, one obtains

$$D=\left[\prod_{i=1}^{N}(1-y_ix)^{-N}\right]\times\left[\sum_{i=0}^{N}F^{(i)}P_i\left(\frac{N(N-1)}{2}+i\right)\right]=0 \ , \tag{2.21}$$

where $P_i(n)$ is a polynomial in $x$ of order $n$. The factor in square brackets must vanish independently and this is equivalent to Eq. (1.1).

To have evaluated the generalized approximant, we would have to solve $3N$ nonlinear equations for the parameters $y_i$, $\gamma_i$ and $A_i$. On the other hand, by the integral-approximant route, we must evaluate the constant coefficients in the polynomials in Eq. (2.21) from systems of linear equations. There are

$$\sum_{i=0}^{N}\left[\frac{N(N+1)}{2}+i+1\right]-1=\frac{N^2(N+1)}{2}+N \tag{2.22}$$

coefficients to determine (since the constant term in $P_N$ can be set equal to 1 without loss of generality), in addition to the $N$ initial conditions which must be satisfied for the differential equation. Clearly the transformation to a linear problem has become costly, in that the number of parameters is now cubic in $N$, instead of linear.

## III. INVARIANCE PROPERTIES

When a Taylor-series expansion of a function is summed directly, each partial sum necessarily diverges at $x=\infty$. The existence of this special point directly effects the shape of the region in the complex plane over which the values of the function can be constructed by this method. When a Taylor series is summed by the method of diagonal Padé approximants, the point $x=\infty$ loses this special significance, and the restriction of the convergence region to a circle centered at the origin is overcome. The proof that the point at infinity, and in fact that no point, other than the origin, is special to the Padé method is based on the invariance of the method under homographic transformations of the form Eq. (1.4). We will concentrate in this section on those integral approximants, described in the Sec. I, which maintain invariance with respect to Eq. (1.4), at least for certain sequences of approximants in the hope that they will be the most powerful ones like the diagonal and near-diagonal sequences of Padé approximants. Substituting Eq. (1.4) into Eq. (1.1) and letting $N$ be $K+2$ plus the sum of the degrees of the polynomials, we see that

$$\sum_{\nu=0}^{K} Q_\nu\left[\frac{Aw}{1+Bw}\right]y^{(\nu)}\left[\frac{Aw}{1+Bw}\right]+R\left[\frac{Aw}{1+Bw}\right]=O(w^N) \ , \tag{3.1}$$

where $y^{(\nu)}$ means $d^\nu y/dx^\nu$, can be form invariant only if, after re-expressing the derivatives with respect to $x$ in terms of those with respect to $w$, the polynomial form of the coefficients can be restored while simultaneously preserving the degrees. We can always make the coefficients of the resultant equation polynomials by multiplying by a suitable power of $(1+Bw)$, but unless special conditions are met, the degrees of the $Q_\nu$'s, and $R$ will be changed. The right-hand side of Eq. (3.1) is not changed in form by this operation. It suffices to compute

$$y^{(1)}=\frac{dy}{dw}(1+Bw)^2/A \ ,$$
$$y^{(2)}=\left[\frac{d^2y}{dw^2}(1+Bw)^4+2B\frac{dy}{dw}(1+Bw)^3\right]\Big/A^2 \ , \tag{3.2}$$

to see that $K\leq 1$ is necessary to obtain an invariance property, as if $Q_2$ is of degree $N_2$, then a factor of $(1+Bw)^{N_2-3}$ is necessary to insure that the coefficient of $dy/dw$ is a polynomial, but the same factor necessarily raises by one the degree of the coefficient of $d^2y/dw^2$. Thus, we find that

$$Q_M(x)y'(x)+P_L(x)y(x)+R_N(x)=O(x^{M+L+N+2}) \ , \tag{3.3}$$

subject to the restriction

$$M=L+2 \ , \quad N=L \tag{3.4}$$

is the most general form of Eq. (3.1) which is invariant with respect to Eq. (1.4). The subscripts now denote the degree of the polynomials.

Equation (3.3) is equivalent, if we expand $y(x)$ in a formal power series in $x$, to a set of linear equations for the coefficients of $Q_M$, $P_L$, and $R_N$. If these coefficients are now used to determine a function $g(x)$ by means of the equations

$$Q_M(x)g'+P_L(x)g+R_N(x)=0 \ , \tag{3.5}$$

$$Q_M(0)=1.0 \ , \tag{3.6}$$

then we call this function the $[N/L;M]$ approximant to $y(x)$. The reason for this notation is that if $Q\equiv 0$, then we have exactly the $[N/L]$ Padé approximant to $g(x)$. The $d$ ln Padé approximant procedure has proven in the past[10] to be a very effective method for analysis of critical phenomena problems. As we have pointed out, approximants defined by Eq. (3.5) are also a direct extension of the $[L/M]$ Padé approximants to $d\ln y/dx$ and would result for $R\equiv 0$. Because of Eq. (3.6) $Q\not\equiv 0$, so, the $[N/L;M]$ are thought of here as direct generalization of the $d$ ln Padé approximants.

## IV. NATURE OF THE APPROXIMANT

We will concentrate our attention on the integral approximant defined by Eqs. (3.3), (3.5), and (3.6). By standard methods we may solve Eq. (3.5) explicitly as

$$g(x)=\exp\left[-\int_0^x\frac{P_L(\xi)}{Q_L(\xi)}d\xi\right]\left[g(0)-\int_0^x\frac{R_N(\eta)}{Q_M(\eta)}\exp\left[\int_0^\eta\frac{P_L(\xi)}{Q_M(\xi)}d\xi\right]d\eta\right] \ . \tag{4.1}$$

Since our goal is the investigation of the singularity structure of certain thermodynamic functions, we will be particularly interested in the behavior of the solution near its singular points. Standard theory shows that the only possible singular points are the zeros of $Q_M$ and $x=\infty$.

In the usual way we can analyze the behavior of Eq. (4.1) at its singular points. Let us write

$$\frac{P_L(x)}{Q_M(x)}=p'(x)+\sum_{i=1}^{M}\frac{\gamma_i}{x-x_i} \ , \tag{4.2}$$

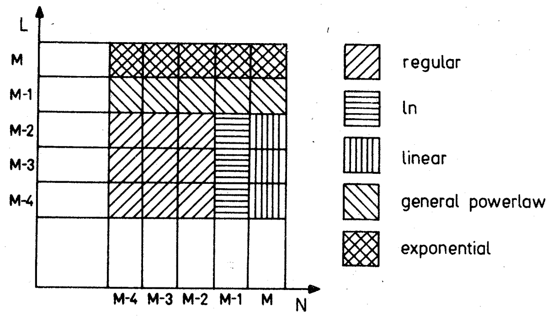


FIG. 1. Map of the divergence behavior at $x=\infty$ for the $[N/L;M]$ integral approximant.

where $p'(x)$ is a polynomial of degree equal to the maximum of zero and $L-M$, and the $x_i$ are the $M$ roots of $Q_M(x)=0$. We assume here that the roots are simple and, consequently, all the finite plane singularities are regular singular points. The parameters $\gamma_i$ are given by

$$\gamma_i = P_L(x_i)/Q_M{}'(x_i) \quad . \tag{4.3}$$

It follows immediately that the first factor of the right-hand side of Eq. (4.1) is

$$\exp\left[-\int_0^x \frac{P_L(\xi)}{Q_M(\xi)}\,d\xi\right] = \exp[-p(x)]\prod_{i=1}^{M}(1-x/x_i)^{-\gamma_i} \quad , \tag{4.4}$$

where $p(x)$ is the integral of $p'(\xi)$ from $\xi=0$ to $\xi=x$. Thus this factor, the solution of the corresponding homogeneous equation, has a power-law behavior at each singular point. The structure of the solution (4,1) for the inhomogeneous equation (3.5) near $x_i$, is given by

$$g(x) = \phi_{1,i}(x)(1-x/x_i)^{-\gamma_i} + \phi_{2,i}(x) \quad , \tag{4.5}$$

except when $\gamma_i$ is a non-positive integer. The functions $\phi_{1,i}(x)$ and $\phi_{2,i}(x)$ are regular in the neighborhood of $x=x_i$.

We can explicitly compute the behavior of $x=\infty$ directly from Eq. (4.1) for various values of $L$, $M$, and $N$. We summarize the results in Fig. 1. The special approximant $[M-2/M-2;M]$ is regular at infinity. The cases $[N/L;M]$ with $L \leq M-2$, $N \leq M-2$ are all regular at infinity but may have certain derivatives with respect to $1/x$ necessarily zero there. If $L \leq M-2$ and $N=M-1$, then the solution (4.1) diverges logarithmically as $x$ goes to infinity. If $L \leq M-2$ and $N > M-1$, then $g(x)$ diverges like $x^{N-M+1}$ as $x\rightarrow\infty$. In the special case $L=M-1$, the polynomial $P(x)$ in Eq. (4.4) vanishes identically, and the dominant behavior at infinity is characterized by

$$c_1 x^{-\sum \gamma_i} + c_2 x^{N-M+1} \quad , \tag{4.6}$$

unless the two exponents are equal, in which case the dominant term is

$$c_3 x^{N-M+1}\ln x \quad . \tag{4.7}$$

For $L > M-1$, the behavior at $x=\infty$ is dominated by the polynomial in Eq. (4.4), and an essential singularity of order $L-M+1$ results.

Since, for applications, we wish to know the parameters, $x_i$, $\gamma_i$, $\phi_{1,i}(x_i)$, and $\phi_{2,i}(x_i)$ corresponding to the singularities, we find it convenient to recase the solution (4.1). To this end let us introduce the notation

$$Q_i(x) = Q_M(x)/(x-x_i) \quad , \tag{4.8}$$

$$P_i(x) = [P_L(x) - \gamma_i Q_i(x)]/(x-x_i) \quad ,$$

then

$$\frac{P_L(x)}{Q_M(x)} = \frac{P_i(x)}{Q_i(x)} + \frac{\gamma_i}{x-x_i} \quad . \tag{4.9}$$

Thus we may rewrite Eq. (4.1) as

$$\begin{aligned} g(x) = {} & \left[1-\frac{x}{x_i}\right]^{-\gamma_i} \exp\left[-\int_0^x \frac{P_i(\xi)}{Q_i(\xi)}\,d\xi\right]\left[g(0) - \int_0^{x_i} \frac{R_N(\eta)}{Q_M(\eta)}\left[1-\frac{\eta}{x_i}\right]^{\gamma_i} \exp\left[\int_0^{\eta} \frac{P_i(\xi)}{Q_i(\xi)}\,d\xi\right]d\eta\right] \\ & + \left[\left[1-\frac{x}{x_i}\right]^{-\gamma_i} \int_x^{x_i} \frac{R_N(\eta)}{Q_M(\eta)}\left[1-\frac{\eta}{x_i}\right]^{\gamma_i} \exp\left[\int_x^{\eta} \frac{P_i(\xi)}{Q_i(\xi)}\,d\xi\right]d\eta\right] \quad , \end{aligned} \tag{4.10}$$

which yields explicit expressions for $\phi_{1,i}(x)$ and $\phi_{2,i}(x)$, provided $\mathrm{Re}\gamma_i > 0$. A different recasting is required otherwise. If we take the limit as $x\rightarrow x_i$, and use Eqs. (4.3) and (4.10), we obtain the expression

$$\phi_{2,i}(x_i) = - R_N(x_i)/P_L(x_i) \tag{4.11}$$

for the remainder, and

$$\phi_{1,i}(x_i)=\exp\left[-\int_0^{x_i} P_i(\xi) \text{ and } Q_i(\xi)\,d\xi\right]\left[g(0)-\int_0^{x_i}\frac{R_N(\eta)}{Q_M(\eta)}\left(1-\frac{\eta}{x_i}\right)^{\gamma_i}\exp\left[\int_0^{\eta}\frac{P_i(\xi)}{Q_i(\xi)}\,d\xi\right]d\eta\right] \quad (4.12)$$

for the amplitude of the singular term.

We remark that if $\gamma_i=1,2,\ldots$, then the separation described in Eq. (4.5) is not well defined, as for any $h(x)$ regular at $x=x_i$, we may also write

$$g(x)=[\phi_{1,i}(x)+(x-x_i)^n h(x)]\,(1-x/x_i)^{-n}+[\phi_{2,i}(x)-h(x)] \ . \quad (4.13)$$

This formula has the consequence that $\phi_{2,i}(x_i)$ is undefined in this case $n=$ positive integer. We will, however, define it by continuity to be the value given by Eq. (4.11).

In order to evaluate numerically Eq. (4.12), we must compute the value of an integral with a singular end point of known type. The integrand behaves like $(1-\eta/x_i)^{\gamma_i-1}$ at the upper end point. As a practical expedient, we have divided the range 0 to $x_i$ into 99 intervals and used Simpson's rule on the first 96 of them. We have used a generalized version of the three-eights rule especially suited to deal with that type end point. Thus, if we let

$$99h=x_i \ ,$$

then we approximate

$$\int_{96h}^{99h}\left(1-\frac{\eta}{x_i}\right)^{\gamma-1}F(\eta)\,d\eta \simeq (3h)^{\gamma}\left\{\left[\frac{1}{\gamma}-\frac{11}{2(\gamma+1)}+\frac{9}{\gamma+2}-\frac{9}{2(\gamma+3)}\right]F(99h) + \left[\frac{9}{\gamma+1}-\frac{45}{2(\gamma+2)}+\frac{27}{2(\gamma+3)}\right]F(98h) + \left[-\frac{9}{2(\gamma+1)}+\frac{18}{\gamma+2}-\frac{27}{2(\gamma+3)}\right] \times F(97h) + \left[\frac{1}{\gamma+1}-\frac{9}{2(\gamma+2)}+\frac{9}{2(\gamma+3)}\right]F(96h)\right\} + O(h^{4+\gamma}) \ . \quad (4.14)$$

This scheme has been adequate to our accuracy requirements for the test cases reported herein. These procedures for the amplitude and remainder calculations are only valid for $\gamma_i > 0$, for, as we mentioned above, a different rearrangement than Eq. (4.10), and, consequently, different formulas from Eqs. (4.11) and (4.12) are required to compute the critical parameters if $\gamma_i \leq 0$.

We remark that in the recent numerical studies of Guttmann[11] of the related "recursion relation" method which revolves around the solution of

$$zQ_M(z)\frac{d^2\psi}{dz^2}+R_M(z)\frac{d\psi}{dz}+S_{M-1}(z)\psi=0 \ , \quad (4.15)$$

instead of Eq. (3.6), the amplitude and remainder calculations were not attempted. In this case, since the point $x=0$ is a singular point [unless $R_M(0)=S_{M-1}(0)=0$, and $Q_M(0)\neq 0$], and there is no simple, explicit, general form of the solution similar to Eq. (4.1), the numerical problem of obtaining the amplitude and remainder is much less straightforward.

There are a fair number of special cases where the above description of the solution (4.1) fails. We mention, for example, that if $\gamma_i=0,-1,-2,-3,\ldots$, then instead of form (4.5) we get

$$g(x)=w_{1,i}(x)\ln(1-x/x_i)(1-x/x_i)^{-\gamma_i}+w_{2,i}(x) \ , \quad (4.16)$$

with the $w_i$'s regular near $x_i$. If $Q_M(x)$ has a double root, then the solution (4.1) can have an essential singularity at that point. (See also Ince[12] and Kamke[13] for a fuller discussion of some of these aspects.) Clearly, a number of other special cases can also arise.

## V. APPLICATION TO TEST SERIES

In order to test the effectiveness of a method for analyzing series expansions, it is necessary to apply it in a controlled situation, i.e., to test functions where one knows the exact behavior. In I, we introduced a set of test functions, chosen to represent a variety of singularity patterns. These test functions are a convenient bench mark and have been used by Guttmann[11] for the sake of comparison. We choose the functions $A-K$ (Table I) to test our integral-approximant method. For a plot of the singularities in these functions see Fig. 2 in I.

The number of approximants one can form for a

TABLE II. Comparison of our integral-approximant IA results with other methods of analysis: (ratio $R$), Padé approximant $P$, generalized approximant $G$, and recurrence reltions $RR$. The parameter tabulated is $\epsilon_n$ for the critical point on the left and for unbiased critical exponent estimates on the right. The main entry under IA is from the most accurate approximant using $\leq n$ terms of the series; an alternate entry in parenthesis represents a more realistic assessment of all the approximants using $n$ terms if the main entry is anomalously precise. Asterisks indicate the method(s) judged to be most successful for each series.

| | | Critical-Point estimates | | | | | | Unbiased-Critical-Exponent Estimates | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $n$ | $R$ | $P$ | $G$ | IA | | RR | $R$ | $P$ | $G$ | IA | | RR |
| $A$ | 10 | 3.2 | 2.7 | | 3.6 | | exact | 2.4 | 1.7 | | 2.8 | | exact |
| | 15 | 8.1 | 4.0 | | 6.2 | | exact | 7.1 | 2.6 | | 4.7 | | exact |
| | 20 | *13.9 | 4.8 | *>10 | 10.1 | (9.0) | exact | *12.8 | 3.0 | *>10 | 8.4 | | exact |
| $B$ | 10 | 2.3 | 2.7 | | 3.9 | | 4.2 | 1.3 | 1.7 | | 3.1 | | 2.9 |
| | 15 | 2.8 | 3.9 | | 6.8 | | 5.4 | 1.6 | 2.5 | | 4.9 | | 3.9 |
| | 20 | 3.1 | 5.1 | 3.5 | *8.9 | | exact | 1.7 | 3.3 | 1.9 | *7.5 | | exact |
| $C$ | 10 | 2.3 | 2.5 | | 4.1 | | 3.2 | 1.0 | 1.2 | | 2.4 | | 1.9 |
| | 15 | 2.5 | 3.4 | | 4.2 | | 4.1 | 1.3 | 2.2 | | 2.6 | | 3.3 |
| | 20 | 2.9 | 4.0 | 3.1 | *7.9 | | exact | 1.4 | 2.4 | 1.5 | *6.2 | | exact |
| $D$ | 10 | 1.7 | 1.9 | | 2.1 | | . . . | 0.8 | 0.7 | | 1.7 | | . . . |
| | 15 | 2.6 | 2.2 | | 4.0 | | 2.0 | 1.4 | 1.0 | | 2.2 | | 0.8 |
| | 20 | 3.6 | 3.5 | *5.4 | 5.3 | (4.9) | 4.0 | 2.0 | 1.9 | *4.3 | 3.6 | | 2.4 |
| $E$ | 10 | 1.6 | 1.3 | | 2.7 | | . . . | 0.7 | 0.4 | | 2.3 | | . . . |
| | 15 | 2.4 | 2.5 | | 3.6 | | 2.0 | 1.3 | 1.4 | | 2.3 | | 0.7 |
| | 20 | 3.0 | 3.7 | 3.8 | *4.8 | | 3.6 | 1.7 | 2.2 | 1.7 | *3.3 | | 2.1 |
| $F$ | 10 | 1.5 | 1.1 | | 1.8 | | 0.9 | 0.8 | 0.3 | | 1.3 | | −0.4 |
| | 15 | 2.8 | 1.4 | | 3.4 | | 1.7 | 1.1 | 0.3 | | 2.8 | | 0.5 |
| | 20 | 3.0 | 2.7 | 2.9 | *5.5 | (4.3) | 5.4 | 1.5 | 1.2 | 1.5 | *3.4 | (2.7) | 2.8 |
| $G$ | 10 | 1.4 | 1.3 | | 1.8 | | 3.2 | 0.6 | 0.4 | | 0.9 | | 1.7 |
| | 15 | 1.6 | 1.3 | | 2.8 | | 2.1 | 0.6 | 0.4 | | 1.8 | | 1.2 |
| | 20 | 1.9 | 2.7 | 2.3 | *4.4 | | 2.0 | 0.9 | 1.3 | 1.2 | *3.9 | (2.3) | 0.7 |
| $H$ | 10 | 1.6 | 1.7 | | 2.5 | | 2.7 | 0.7 | 0.7 | | 1.9 | | 2.5 |
| | 15 | 2.0 | 1.8 | | 3.0 | | 2.8 | 0.9 | 0.9 | | 2.6 | | 1.7 |
| | 20 | 2.2 | 2.4 | 2.5 | *3.4 | (2.6) | 2.0 | 1.3 | 1.3 | 1.7 | *2.6 | (1.6) | 1.2 |
| $I$ | 10 | 1.0 | 0.9 | | 3.3 | | 2.0 | 0.1 | −0.4 | | 1.2 | | 0.9 |
| | 15 | 1.2 | 1.4 | | 3.3 | | 1.7 | 0.1 | 2.3 | | 2.1 | | 0.8 |
| | 20 | 1.5 | 2.2 | 1.6 | *3.3 | (2.4) | 2.6 | 0.4 | 1.3 | 0.4 | *2.1 | (1.7) | 1.5 |
| $J$ | 10 | 1.1 | 2.2 | | 3.7 | | exact | 0.2 | 1.4 | | 3.0 | | exact |
| | 15 | 1.7 | 3.5 | | 7.1 | | exact | 0.5 | 2.2 | | 5.2 | | exact |
| | 20 | 2.0 | 4.4 | 7.2 | *8.7 | (8.0) | exact | 0.8 | 2.7 | 6.3 | *7.4 | (6.7) | exact |
| $K$ | 10 | 1.1 | 0.7 | | 3.4 | | 2.4 | 0.1 | 0.1 | | 1.7 | | 1.2 |
| | 15 | 1.7 | 3.0 | | 5.2 | | 3.2 | 0.5 | 1.7 | | 3.8 | | 1.9 |
| | 20 | 2.0 | 3.9 | 6.5 | *6.9 | | 5.3 | 0.8 | 2.3 | 5.5 | 5.5 | | 3.4 |

TABLE III. Comparison of our integral-approximant IA results with other methods. The parameter tabulated is $\epsilon_n$ for biased critical exponent estimates. See Table II caption for further details.

| | $n$ | Biased-Critical-Exponent Estimates $R$ | $P$ | IA | | RR |
|---|---|---|---|---|---|---|
| $A$ | 10 | 4.1 | 2.4 | 3.1 | | exact |
| | 15 | 9.4 | 3.0 | 7.1 | | exact |
| | 20 | *15.4 | 3.6 | 10.1 | (9.0) | exact |
| $B$ | 10 | 1.7 | 2.7 | 3.5 | | 3.4 |
| | 15 | 1.9 | 3.3 | 5.9 | | 4.6 |
| | 20 | 2.0 | 3.7 | *9.9 | (8.6) | exact |
| $C$ | 10 | 1.3 | 1.7 | 2.7 | | 1.9 |
| | 15 | 1.5 | 2.4 | 4.6 | | 3.3 |
| | 20 | 1.6 | 3.1 | *7.5 | (6.9) | exact |
| $D$ | 10 | 1.5 | 1.0 | 2.2 | | ... |
| | 15 | 2.6 | 1.9 | 3.9 | | 0.8 |
| | 20 | 3.7 | 2.3 | *4.7 | (3.8) | 2.4 |
| $E$ | 10 | 1.6 | 1.3 | 3.5 | | ... |
| | 15 | 1.8 | 1.8 | 3.5 | | 0.7 |
| | 20 | 2.0 | 2.4 | *4.7 | (4.0) | 2.1 |
| $F$ | 10 | 0.8 | 0.4 | 2.1 | | −0.4 |
| | 15 | 1.3 | 1.2 | 3.4 | | 0.5 |
| | 20 | 1.6 | 1.8 | *4.1 | (3.5) | 2.8 |
| $G$ | 10 | 1.3 | 0.8 | 2.0 | | 1.7 |
| | 15 | 1.4 | 1.1 | 2.2 | | 1.2 |
| | 20 | 1.5 | 2.0 | 2.2 | (1.6) | 0.7 |
| $H$ | 10 | 1.5 | 0.9 | 2.9 | | 2.5 |
| | 15 | 1.6 | 1.2 | 2.9 | | 1.7 |
| | 20 | 1.6 | 1.7 | 3.0 | (1.6) | 1.2 |
| $I$ | 10 | 0.8 | 0.6 | 2.7 | | 0.9 |
| | 15 | 0.8 | 0.8 | 2.7 | | 0.8 |
| | 20 | 1.2 | 1.7 | 3.3 | (1.6) | 1.5 |
| $J$ | 10 | 0.7 | 1.7 | 3.9 | | exact |
| | 15 | 1.2 | 2.7 | 6.1 | | exact |
| | 20 | 1.4 | 3.2 | *9.3 | (8.0) | exact |
| $K$ | 10 | 0.7 | 1.4 | 3.4 | | 1.2 |
| | 15 | 1.2 | 2.0 | 4.8 | | 1.9 |
| | 20 | 1.4 | 2.5 | *6.7 | (6.0) | 3.4 |

function using up to 20 terms of the series is very large. Because of the invariance property for the $[M-2/M-2;M]$ approximant and the variety of behaviors at $x=\infty$ exhibited by approximants in the $5\times 5$ blocks centered on the $[M-2/M-2;M]$ (see Fig. 1) we have chosen to do the analysis using only those approximants, i.e.,

$$[M-i/M-j;M]\ ,\quad 0\leq i,j\leq 4\ . \tag{5.1}$$

To compare the data with methods considered in I and II, we use the first 20 terms in the expansions of the test series. This allows us to form approximants of the form (5.1) with $M\leq 8$.

We have calculated unbiased estimates for the location of the physical singularity $x_1$ and the exponent $\gamma_1$, using Eqs. (4.2) and (4.3). In Table II the results of this analysis (IA) are compared with the ratio method $R$, Padé-approximant method (using logarithmic derivatives) $P$, the generalized approximants $G$, defined in Eq. (2.28) of II, and the integral approximants from a second-order homogeneous differential equation [Eq. (1.1), with $K=2$] used by Guttmann[11] and called, by him, the recurrence relation (RR) method.

The quantity tabulated is

$$\epsilon_n=-\log_{10}\left|\frac{p_n-p_{\text{exact}}}{p_{\text{exact}}}\right|\ , \tag{5.2}$$

where $p_n$ is the best estimate of the critical parameter $p$ using $n$ terms of the series. In Table II, the critical parameter $p$ represents the principal singularity $x_1$ or $x_c$ in the left columns and the corresponding exponent $\gamma_1$, or simply $\gamma$, in the right columns. Guttmann points out that functions $A$, $B$, and $J$ (also $L$, which is not included in our present analysis) can be determined exactly by the RR method using 10 terms in the series expansion for each. It appears to us that this statement is correct for functions $A$ and $J$, i.e., that they exactly satisfy Eq. (1.1), with $K=2$, and that 10 series coefficients are necessary to determine the appropriate coefficients in the polynomials $Q_\nu(x)$. It is also true for $L$, but only 7 series coefficients are required. However, for $B$, *and also for C*, the equation is satisfied exactly, but 16 series coefficients are required to evaluate the $Q_\nu(x)$. Guttmann (private communication) has agreed with this analysis.

The proof that $A$ satisfies the equation is as follows: for series $A$, we have directly

$$f=(1-x)^{-1.5}+e^{-x}\ ,\quad f'=\tfrac{3}{2}(1-x)^{-2.5}-e^{-x}\ ,$$
$$f''=\tfrac{15}{4}(1-x)^{-3.5}+e^{-x}\ . \tag{5.3}$$

By direct computation we find

$$(1-x)(\tfrac{5}{2}-x)f''-(\tfrac{11}{4}+2x-x^2)f' + (\tfrac{3}{2}x-\tfrac{21}{4})f=0 \tag{5.4}$$

for series $A$. By the usual theory of differential equations, we know that test series $A$ must be given as the solution of Eq. (5.4), determined by the initial conditions

$$f(0)=2\ ,\quad f'(0)=0.5\ . \tag{5.5}$$

The proof for the other series is similar, and the equations can be found by writing the first and second derivatives as a rational factor times each non-rational term in the function, and then using standard algebra to form a combination which is independent of the non-rational terms.

Because we allow the order of the polynomials in Eq. (1.2) to vary over a much wider range than does the RR method, we have several approximants using a given number of terms in the series. The values of $\epsilon_n$ tabulated under the IA column heading are obtained from the most accurate approximant using $\leq n$ terms of the series. Usually the other approximants have converged sufficiently that the value quoted is a fair one. In those cases where the best estimate is anomalously accurate, we quote in brackets a more realistic value which we feel more fairly represents the accuracy of the method.

In the discussion that follows, the cases where the RR method is exact are excluded from the comparison.

It is apparent from Table II that the integral-approximant procedure is nearly always at least as good as any other non-exact method. In fact, for functions $B$ and $C$ integral approximants give nearly 4 more significant figures than does the Padé method, the best of the other three. For functions $E$ and $G$ we find integral approximants are significantly better than the other four methods, and for $F$ integral approximants and the recurrence relation method are similar but both much better than the other three methods. For functions $J$ and $K$ there is evidence that integral approximants are slightly better than the generalized approximant scheme, but both are significantly better than the traditional ratio and Padé procedures. For function $A$, the ratio and generalized approximant methods do better than integral approximants, and for $D$ the generalized approximants do better than integral approximants. For $G$ and $H$ all methods are poor; but interestingly the integral and recurrence relation approximants show little or no improvement as additional terms are used. This remark will be relevant to some observations we will make about the analysis of the low-temperature Ising susceptibility series.

It is possible to modify the integral-approximant scheme by forcing the approximant to have a singularity at $x=x_c$ and thereby obtain biased estimates for the critical exponent at the singularity. In the $[N/L;M]$ approximant the polynomial

$$Q_M(x)=1+q_1x+q_2x^2+\cdots+q_Mx^M$$

is replaced by

$$Q_M{}^*(x) = \left(1 - \frac{x}{x_c}\right)(1 + q_1{}^*x + q_2{}^*x^2 + \cdots + q_{m-1}{}^*x^{M-1}) \ .$$

There is now one fewer unknown coefficient, hence the fixed singularity approximant will use one less series coefficient than the regular approximant of the same order.

In Table III results of the analysis of the test series using fixed singularity integral approximants are compared with biased estimates of the critical exponent obtained from other methods. The same qualifications apply to the entries in the IA column as applied in Table II. Again, we exclude from the discussion the 4 cases where RR is exact. For functions $B$, $C$, $J$, and $K$, the IA approximants predict $\gamma$ with 3–6 significant figures additional accuracy. For $D$, $E$, and $F$, we also find IA is more effective but not so decisively. The functions $G$, $H$, and $I$ are not amenable to analysis by any of the methods considered; all seem equally unsuitable, and again we observe the tendency in IA and RR for there to be essentially no improvement as many additional series terms are used.

## VI. APPLICATION TO ISING LOW-TEMPERATURE SUSCEPTIBILITY

One of the principal motivations for devising new methods of analyzing series is to improve the estimation of the critical exponents for the low-temperature three-dimensional Ising-model series. Scaling theory

TABLE IV. Biased estimates of $\gamma'$ for the low-temperature Ising susceptibility on the bcc lattice using $[N/L;M]$ integral approximants, tabulated by number of series coefficients used.

| | | | bcc | | |
|---|---|---|---|---|---|
| No. terms used | 19 | 20 | 21 | 22 | 23 |
| | 1.3356 | 1.2987 | 1.3271 | 1.3032 | 1.2463 |
| | 1.3153 | 1.3267 | 1.3289 | (0.0061)[b] | |
| | 1.3550 | 1.3130 | | (0.7581)[b] | |
| | 1.3561 | 1.3314 | | | |
| | 1.3484 | (1.1444)[b] | | | |
| | 1.3493 | (0.9586)[b] | | | |
| | 1.3603 | | | | |
| | 1.3304 | | | | |
| No. defects[a] | 1 | 2 | 6 | 6 | 7 |
| Average | 1.3438 | 1.3175 | 1.3280 | 1.3032 | 1.2463 |

| | | | | |
|---|---|---|---|---|
| No. terms used | 24 | 25 | 26 | 27 |
| | 1.2316 | 1.2330 | 1.2488 | 1.2562 |
| | 1.2293 | 1.3123 | 1.2629 | 1.2555 |
| | 1.2816 | 1.2750 | 1.2526 | 1.2388 |
| | 1.2512 | 1.2576 | 1.2616 | 1.2537 |
| | | | 1.2580 | 1.2247 |
| | | | 1.2847 | 1.2650 |
| | | | 1.2592 | |
| No. defects[a] | 4 | 5 | 1 | 2 |
| Average | 1.2484 | 1.2695 | 1.2611 | 1.2490 |

[a]Number of approximants containing "defects." See I.

[b]Interference caused by presence of a singularity on positive real axis slightly beyond physical singularity. These values are excluded from averages.

TABLE V. Biased estimates of $\gamma'$ for the low-temperature Ising susceptibility on the fcc, sc, and $D$ lattices using $[N/L;M]$ integral approximants, tabulated by number of series coefficients used.

| fcc No. terms used | 30 | 31 | 32 | 33 | 34 | 35 |
|---|---|---|---|---|---|---|
| | | 1.3771 | 1.2489 | 1.2390 | 1.2381 | 1.2413 |
| | | 1.3721 | 1.3641 | 1.2937 | 1.2382 | 1.2885 |
| | | 1.3747 | 1.3215 | 1.2871 | 1.3026 | 1.2433 |
| | | 1.2898 | 1.3131 | 1.3048 | 1.3068 | 1.2429 |
| | | 1.3631 | 1.3305 | | 1.2367 | (1.1276)[b] |
| | | 1.2922 | 1.2589 | | 1.2801 | 1.2545 |
| | | | | | (1.0272)[b] | |
| | | | | | 1.2776 | |
| No defects[a] | | 3 | 2 | 4 | 1 | 2 |
| Average | | 1.3448 | 1.3062 | 1.2812 | 1.2686 | 1.2541 |

| sc No. terms used | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| | 1.3423 | 1.2567 | 1.2476 | 1.4108 | 1.2586 | 1.1833 |
| | 1.3387 | 1.3101 | 1.3311 | (1.1123)[b] | 1.3955 | 1.3675 |
| | 1.3238 | 1.3309 | 1.3339 | | 1.2038 | |
| | 1.3186 | 1.3437 | 1.2217 | | 1.2584 | |
| | 1.3389 | 1.3146 | 1.3084 | | | |
| | 1.1925 | | 1.2901 | | | |
| | 1.3417 | | | | | |
| No defects[a] | 2 | 3 | 2 | 7 | 4 | 6 |
| Average | 1.3138 | 1.3112 | 1.2888 | 1.4108 | 1.2791 | 1.2754 |

| D No. terms used | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|
| | 1.5148 | 1.4521 | 1.2316 | 1.2129 | 1.2668 | 1.2773 |
| | 1.5092 | 1.3659 | 1.1867 | 1.1938 | 1.2626 | 1.2560 |
| | 1.3957 | 1.4310 | 1.0699 | 1.2311 | 1.2616 | 1.2973 |
| | 1.4338 | 1.4309 | 1.3519 | 1.2462 | 1.2431 | 1.2728 |
| | 1.4128 | 1.4038 | 1.2843 | 1.2556 | 1.2472 | 1.2943 |
| | 1.4168 | 1.4309 | | 1.2667 | 1.3120 | 1.2956 |
| | | 1.4301 | | 1.1697 | 1.2713 | 1.2517 |
| | | | | | 1.2469 | |
| No defects[a] | 0 | 0 | 3 | 1 | 1 | 1 |
| Average | 1.4472 | 1.4207 | 1.2249 | 1.2251 | 1.2639 | 1.2779 |

[a]Number of approximants containing "defects." See I.

[b]Interference caused by presence of a singularity on the positive real axis slightly beyond the physical singularity. These values are excluded from averages.

suggests that the low-temperature exponents should equal the corresponding high-temperature exponents ($\alpha'=\alpha$, $\gamma'=\gamma$, $\nu'=\nu$). This symmetry is implicit in all the applications of the renormalization-group techniques to critical phenomena. However, for the Ising model, all series expansion studies of the susceptibility $\chi$ have shown quite poor convergence of estimates for $\gamma'$, but nevertheless, a tendency for the $\gamma'$ estimates to be greater than those for $\gamma$. On the basis of series evidence, alone, one would conclude $\gamma' \geqslant \gamma$. The extent of the discrepancy between $\gamma'$ and $\gamma$ in most studies seems to be lattice dependent, strongly indicating that the method(s) of analysis used is not able to adequately fit enough of the structure in the low-temperature function. The number and location of additional singularities in the low-temperature $\chi$ series is known to be lattice dependent; there are 4, 2, 1, and 0 singularities closer to the origin than the Curie point on the fcc, bcc, sc, and diamond ($D$) lattices, respectively. Hence it is hoped that new methods can be devised which will fit the structure of the low-temperature functions and thereby produce well-converged estimates of $\gamma'$, etc., which will either agree with the scaling predictions, or show a clear difference from them.

In our analysis of the low-temperature Ising susceptibility series on three-dimensional lattices, we have observed a rather striking onset of convergence in the $\gamma'$ estimates toward the high-temperature exponent value $\gamma=1.25$. This effect is most apparent in the data for the bcc lattice. In Table IV are tabulated in separate columns the biased exponent $\gamma'$ estimates from the $[N/L;M]$ integral approximants which use a given number of terms in the series. At the end of the table, we have used the 32-term expansion of Elliott.[14] From the Table it is evident that at term 23 or 24 the estimates of $\gamma'$ suddenly drop from values above 1.30 to values very close to 1.25. The estimates using from 28 to 32 terms are also close to 1.25, although there tends to be a large number of approximants in this range containing defects (see I).

In Table V we give similar tabulations for the fcc, sc, and diamond lattices. Here we use the series of Sykes *et al.*[15] The last column in this table uses the last published term in the series expansion. For the fcc lattice there is evidence that the estimates are just reaching the onset of convergence to values close to 1.25. One might conclude that the onset occurs at term 34 or 35. For the sc, although one estimate at term 17 and both at term 18 are poor, there are, nevertheless, three good estimates at term 17 that suggest this might be the onset. For the diamond lattice, in spite of the short length of the series, the onset appears quite sharply at term 11.

It is instructive to compare the number of singularities in $\chi$ which are less than, or equal to, the distance of the Curie point from the origin of the complex $u$ plane ($u=e^{-4J/kT}$ is the low-temperature expansion variable), with the number of series terms which must be used to just observe the onset of agreement between $\gamma'$ and $\gamma$. This is done in Table VI.

TABLE VI. Dependence of onset of agreement between $\gamma'$ and $\gamma$ on number of series coefficients used calculating the integral approximant.

| Lattice | $D$ | sc | bcc | fcc |
|---|---|---|---|---|
| Number of singularities ($n$) | 1 | 2 | 3 | 5 |
| Number of terms to observe onset | 11 | 17 | 23 | 34 |
| $5+6n$ | 11 | 17 | 23 | 35 |

It is suggestive that, for every additional singularity in the function, one requires 6 additional series terms in order for the integral approximants to accommodate the additional structure. The "order" of an integral approximant may be said to have increased by one when the order of each of the polynomial coefficients (1.2) increases by one. For the first-order inhomogeneous case, this increase requires three additional terms in the series. Hence an additional singularity requires an increase of two in the order of the approximant, one to accommodate the singularity itself and one to accommodate the additional "valley" which is created.

The bcc lattice, by virtue of the large number of terms available relative to the number of singularities near the origin, gives the strongest evidence of the agreement between $\gamma'$ and $\gamma$. However, we believe that the integral-approximant method has given us some insight into the difficulty with low-temperature Ising series and that although the expansions for the other lattices are not known much beyond the threshold of the convergence we seek, they agree with the bcc result and support our case that direct series expansion evidence is now consistent[16] with $\gamma'=\gamma$.

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