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Methods of Series Analysis. II. Generalized and Extended Methods with Application to the Ising Model*

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Several new general methods of series analysis are introduced and tested on an assortment of known functions. These methods are then applied to several of the series expansions known for the thermodynamic properties of the spin-$\frac{1}{2}$ Ising model. We are able to obtain an *unbiased* analysis of the high-temperature specific-heat singularity, and find $\alpha \approx 0.13 \pm 0.01$. The application of our methods in other cases generally agrees with that of previous workers. Our methods in practice amount to procedures for looking more closely at the dominant singularity, at the expense of accuracy for competing singularities. For certain types of function, thought to occur in the study of critical phenomena, our methods are noticeably more effective than those previously employed.

I. INTRODUCTION AND SUMMARY

Although many accurate estimates for the location of singularities and the exponents with which these divergences occur have been made from series expansions for the thermodynamic properties of a system, there are also many instances where accurate predictions of these parameters have been impossible using current methods of series analysis. The reasons for obtaining poor results are not fully understood but certainly include the failure of the analysis to properly account for all interfering singularities, and probably also include the fact that the form of the function may not correspond to that functional form presupposed by the method of analysis. This question has been investigated by Hunter and Baker[1] (hereinafter referred to as I) and the examples considered there illustrate the effect of other singularities and the form of the function on the accuracy of the analysis.

In this paper we introduce several new, quite general methods of analyzing series expansions. These methods are ideally suited to analyze functions of the form

$$F(x) = \sum_{i=1}^{N} A_i (1 - y_i x)^{-\gamma_i} . \tag{1.1}$$

This seems a logical form to consider since the Padé-approximant procedures, best suited to the form

$$F(x) = A(x) \prod_{i=1}^{N} (1 - y_i x)^{-\gamma_i} , \tag{1.2}$$

although very helpful do not give the desired precision for some physical functions (e.g., Ising low-temperature susceptibility and specific heat) and for some of the functions considered in I. The form (1.1) is not as general as that proposed by Thompson *et al.*,[2] but their analysis which followed was equivalent to assuming the form (1.2) (see I). Our new methods offer an alternative for functions not of the form (1.2). Of course, the ratio method does not presuppose that the dominant singularity factors but, as it is capable of approximating only one singularity, it is ineffective when there is interference by other singularities regardless of their form.

Two of our new methods are designed to detect function forms which, although quite general in themselves, are special forms of (1.1). We also consider the completely general case of (1.1), and finally we modify that procedure to admit the even more general case where to the right-hand side of (1.1) one adds any function of x which in our analysis is approximated by a Padé-approximant-like term.

The first method described in Sec. II is applicable to the case where $\gamma_i = \gamma$ for all i in (1.1) and where an accurate estimate of γ is available. (For the low-temperature Ising susceptibility the exponents for all of the singularities closer to the origin than the physical singularity $(1 - T/T_c)^{-\gamma'}$ are very close to γ'.) The binomial coefficient $\binom{-\gamma}{j}$ is, for this case, a factor of the series coefficient a_j, so if the appropriate such factor is divided out of each known series coefficient, one obtains the series for a renormalized function whose singularities are now simple poles. One may then form Padé approximants directly to the renormalized series to deduce the location and amplitudes of the singularities.

The second method is appropriate to detect confluent singularities in a function, and is ideally suited to (1.1) with $y_i = y$ for all i when an accurate estimate for y is available. No other method of analysis of which we are aware will detect confluence to this degree of generality. In Sec. II B we derive a transformation which when applied to a function of the required form results in a func-

tion whose poles (simple) have the same value as the exponents in the original function. Our procedure is also useful for studying functions modified by the presence of an additive or multiplicative function which is analytic at $x=y^{-1}$, since when expanded in a Taylor series about $x=y^{-1}$ the function has the form of an infinite sum of confluent singularities.

In our procedure for treating the general case (1.1) with no restrictions, one calculates a set of estimates for the $3N$ parameters A_i, y_i, and γ_i, $i=1, \ldots, N$, by requiring that exactly $3N$ coefficients in the expansion of the right-hand side of (1.1) agree with the corresponding coefficients in the given series. The conditions so imposed are nonlinear in the parameters y_i and γ_i, and the solution of the equations is a difficult numerical problem. The method and the difficulties which arise are discussed in Sec. II C. The generalization to include a Padé-approximant-like term makes the method applicable to a more general class of functions than (1.1) and in some cases it permits us to obtain reasonable approximants to a series using fewer general branch-point singularities. The generalized approximants are characterized by parameters N, D, and M, which are, respectively, the number of branch-point singularities of the form (1.1) and the order of the denominator and numerator in the additive Padé term. The case $D=0$ corresponds to the procedures described in Sec. II C, and varying M merely determines which block of $3N$ coefficients is used in calculating A_i, y_i, and γ_i. This generalized procedure is discussed in Sec. II D.

We have applied these methods to several test functions including those used in I in studying the previously available methods. For the first two methods we find the analysis is straightforward and the results agree with what we would expect to see on theoretical grounds. In applying the most general form of analysis we occasionally find it difficult or impossible to solve for a particular approximant. In particular, for given N, it becomes very difficult to obtain solutions for large D and our tables have not yet been extended to include such approximants. However, the evidence is quite clear that for functions close to the form (1.1) our general method provides more accurate estimates of the critical parameters (up to three more significant figures) than do the methods described in I. For those functions where the dominant branch point is multiplied by some function of x we found, as expected, that the standard procedures were as good as or better than the new method.

Finally, in Sec. IV, we apply the new methods to some spin-$\frac{1}{2}$ Ising-model series. The analysis of the low-temperature-susceptibility series using the exponent-renormalization procedures indicates that although the exponents of the nonphysical singularities are probably all equal to one another and close to γ', they probably do not equal γ'. We also conclude, on the basis of negative results using the confluent-singularity method, that the present imprecise results for the Ising low-temperature functions are probably not due to a confluence of singularities.

Although the application of the confluent-singularity method to the high-temperature specific-heat series gave no indication of confluence, the Padé analysis of the transformed series did provide a biased table of estimates for α. We found these to be in excellent agreement with the best biased-ratio sequences[3] for the three-dimensional lattices we studied.

We have applied the most general method to two high-temperature series and to the low-temperature susceptibility. For the high-temperature susceptibility the estimates of all the parameters assuming $N=1$ are very smoothly behaved. The estimates for γ are consistently just a little below the best estimates using Padé approximants and ratios (~ 1.246 vs 1.250). This deviation is probably due to the assumed additive form, and we do not suggest any revision to previous conclusions. For the high-temperature specific heat, our results which are unbiased by any assumed value for the critical point y indicate that the exponent

$$\alpha = 0.13 \pm 0.01 \ .$$

This is in good agreement with the accepted value $\alpha=\frac{1}{8}$ due to Sykes *et al.*,[3] whose published sequences of estimates depend upon the choice of y. Our results represent a more complete set of unbiased estimates than are obtainable by the unbiased-ratio procedure [Eq. (2.7) of I].

The low-temperature susceptibility on the sc lattice has two important branch points which we have tried to study using $N=2$ in our general procedure. Owing to numerical problems we are unable to reach a conclusion concerning the amenability of this function to this type of analysis. The evidence indicates that if the form we assume is reasonable, then either there are more singularities beyond the Curie point which must be accounted for by increasing N, or else we need higher-order denominators in the Padé-type term to better approximate the corrections to (1.1).

II. SERIES-ANALYSIS METHODS

A. Exponent Renormalization

We shall first consider analytic procedures appropriate when the form of the function is a restricted case of Eq. (1.1). In the first instance we consider the case where all the γ_i's are equal and

where a reliable estimate of their common value—say, γ—is available. We shall refer to this procedure as the equal exponent or *exponent-renormalization* procedure. For the restricted form

$$F(x)=\sum_{i=1}^{N} A_i(1-y_i x)^{-\gamma}\,, \tag{2.1}$$

the expansion coefficients have the form

$$a_j=\sum_{i=1}^{N} A_i\binom{-\gamma}{j}(-y_i)^j\,, \tag{2.2}$$

where the binomial coefficient $\binom{-\gamma}{j}$ is now a factor of a_j. We wish to consider the auxiliary function $\mathfrak{F}(x)$ whose expansion coefficients have the form

$$a_j^*=\sum_{i=1}^{N} A_i(-y_i)^j$$

and are obtained by dividing the coefficients of the original function by $\binom{-\gamma}{j}$. $\mathfrak{F}(x)$ has the form

$$\mathfrak{F}(x)=\sum_{j=0}^{\infty}\sum_{i=1}^{N} A_i(-y_i)^j x^j=\sum_{i=1}^{N}\frac{A_i}{1+y_i x}\,. \tag{2.3}$$

The auxiliary function has simple poles (rather than branch points) located at $x=-y_i^{-1}$; the residue at each of these poles is A_i/y_i. The auxiliary function is of the form of an $[N-1/N]$ Padé approximant.

The series-analysis procedure we propose for situations where it is reasonable to assume that the function the series represents may be of the form (2.1) or at least closely approximated by it, is to form an auxiliary series by dividing the coefficients a_j by binomial coefficients $\binom{-\gamma}{j}$, form Padé approximants, particularly $[n-1/n]$ approximants, directly to the auxiliary series, and examine the roots and residue of these approximants.

If the index of one of the singularities—say, on the real axis—is not exactly the value chosen for renormalization, then the Padé approximant to the auxiliary function will contain an alternation of poles and zeros spreading outward along the real axis from the expected location of the singularity. This type of pattern is the way in which a Padé approximant will approximate a branch cut in a function. The residue of the branch point (end point of the cut) may no longer give a reliable estimate of the amplitude of the singularity in the original function.

B. Confluent-Singularity Analysis

The second restricted case applies to the case of confluent singularities, i.e., to

$$F(x)=\sum_{i=1}^{N} A_i(1-yx)^{-\gamma_i}\,, \tag{2.4}$$

where all the singularities of (1.1) are restricted to fall at $x=y^{-1}$. Usual Padé-approximant procedures are only capable of detecting the strongest such singularity. Correction terms to the ratio equations have been calculated for the case of two confluent singularities[4] but simultaneous solution for the two exponents is very difficult; rather, one may calculate the location and the secondary exponent given the primary exponent. For our procedure using Padé approximants, one may estimate any number of exponents associated with confluent singularities *given the location.*

From (2.4) we form an auxiliary function $\mathfrak{F}(\xi)$ in two steps. First we expand (2.4) in the variable ξ,

$$f(\xi)\equiv F(x(\xi))=\sum_{i=1}^{N} A_i e^{-\gamma_i \ln(1-yx)}$$

$$=\sum_{i=1}^{N} A_i e^{\gamma_i \xi}=\sum_{i=1}^{N}\sum_{k=0}^{\infty}\frac{A_i\gamma_i^k\xi^k}{k!}\,, \tag{2.5}$$

where

$$x=y^{-1}(1-e^{-\xi})\,. \tag{2.6}$$

Now multiply the kth coefficient in the expansion by $k!$ to obtain the expansion of $\mathfrak{F}(\xi)$,

$$\mathfrak{F}(\xi)=\sum_{i=1}^{N}\sum_{k=0}^{\infty} A_i\gamma_i^k\xi^k\,, \tag{2.7}$$

and performing the k summation,

$$\mathfrak{F}(\xi)=\sum_{i=1}^{N}\frac{A_i}{1-\gamma_i\xi}\,. \tag{2.8}$$

The auxilary function $\mathfrak{F}(\xi)$ has simple poles at $\xi=1/\gamma_i$ and residues $-A_i/\gamma_i$, all of which may be determined from the Padé approximants to $\mathfrak{F}(\xi)$.

Using the simple integral identity

$$\int_0^{\infty} e^{-t}t^n\,dt=n!\,, \tag{2.9}$$

we note that the transformation from $f(\xi)$ to $\mathfrak{F}(\xi)$ can be expressed as

$$\mathfrak{F}(\xi)=\int_0^{\infty} e^{-t}f(t\xi)\,dt=(1/\xi)\,\mathfrak{L}(1/\xi) \tag{2.10}$$

$$=\int_0^{\infty} e^{-t}F(y^{-1}(1-e^{-t\xi}))\,dt\,, \tag{2.11}$$

where $\mathfrak{L}(s)$ is the Laplace transform of $f(z)$. The complete transformation (2.11) from $F(x)$ was obtained by substitution of (2.5) into (2.10). Since we then approximate $\mathfrak{F}(\xi)$ by a Padé approximant, we may then formally obtain the approximant to $F(x)$ using the inverse transformation

$$F(x)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{1}{p}\,\mathfrak{F}\left(\frac{1}{p}\right)e^{-p\ln(1-yx)}\,dp\,, \tag{2.12}$$

where the constant c must be chosen greater than the maximum of the real parts of the γ_i, i.e., so that the line $\mathrm{Re}(p)=c$ may be the right-hand boundary of a contour in the p plane which encloses all the singularities $p=\gamma_i$. However, this is equivalent to writing

$$F(x)\approx\sum_{i=1}^{N} A_j(1-yx)^{-\gamma_i} \tag{2.13}$$

directly from the roots and residue of the Padé ap-

proximant.

We therefore have a procedure for detecting confluence in the singularity structure of a series if it is reasonable to assume that the form of the function the series represents is close to (2.4). We apply the transformation defined by (2.5) and (2.10) to the series for $F(x)$ and form Padé approximants to the transformed series. If $F(x)$ were exactly of the form (2.4), then the approximant $[N-1/N]$ would exactly represent the transformed function. Exponent values close to zero will be difficult to detect because in the transformed function they appear as poles that are well away from the origin and hence are poorly approximated in the Padé approximant.

This procedure has the added advantage of being able to represent quite accurately functions of the forms

$$F(x)=(1-yx)^{-\gamma}g(x) \tag{2.14}$$

and

$$F(x)=A(1-yx)^{-\gamma}+g(x)\,, \tag{2.15}$$

where $g(x)$ is analytic at $x=y^{-1}$, provided a sufficient number of terms in the expansion of $F(x)$ are available. With $g(x)$ expanded as a Taylor series about $x=y^{-1}$, the form of (2.14) and (2.15) is the same as (2.4) with $N=\infty$. Finite-order Padé approximants $[n-1/n]$ then represent $F(x)$ in a truncated form.

The location of the poles of interest in the transformed function is found to be quite insensitive to errors in the estimation of y. If for a particular singularity the value of y used in the transformation differs from the true value by Δy, then we observe that the error of the $[m+1/m]$ Padé approximant in the estimated exponent is of order $(\gamma_1+2m)(\Delta y/y)$, while the error in the amplitude is of order $(\gamma_1+2m)\ln(\gamma_1+2m)(\Delta y/y)$. In principal, however, if we pick too large a value for y, there will be no real positive pole, but a pair of complex singularities in the ξ plane. If, on the other hand, we select slightly too small a value for y, a cut on the entire positive real ξ axis is required.

If we define $\mathfrak{F}(\xi)$ by (2.11), which is valid for any formal power series $F(x)$, then by the integral representation, and by contour rotation, if $F(x)$ is continuous on $0\le x<y^{-1}$ and diverges no faster than $A(1-xy)^{-\gamma}$ at $x=y^{-1}$, then $\mathfrak{F}(\xi)$ is regular in $|\gamma\xi-\frac{1}{2}|<\frac{1}{2}$. Of course, many times $\mathfrak{F}(\xi)$ will be analytic in a wider domain than this minimal one.

C. General Analysis for Additive Singularities

The general case, where we consider Eq. (1.1) and do not specialize any of the parameters or assume accurate prior knowledge of any of them, is much more difficult to treat. If there are N terms in the right-hand side of (1.1), we seek a scheme to simultaneously estimate the unknown parameters A_i, y_i, and γ_i for $i=1,\ldots,N$. We may choose these parameters so that any $3N$ coefficients in the expansion of (1.1) agree exactly with the corresponding $3N$ coefficients in the actual expansion we are dealing with. In fact, we solve the equation

$$\sum_{i=1}^{N}\frac{A_i}{\gamma_i}\binom{-\gamma_i}{j}(-y_i)^j=a_j\,,\quad j=J,J+1,\ldots,J+3N-1\,,\quad J\neq 0, \tag{2.16}$$

where we have modified the assumed form (1.1) to become

$$F(x)=A_0+\sum_{i=1}^{N}\frac{A_i}{\gamma_i}\left[(1-y_ix)^{-\gamma_i}-1\right], \tag{2.17}$$

so that the possibility of a logarithmic singularity of the form

$$A_k\ln(1-y_kx) \tag{2.18}$$

is included in (2.17) in the limit $\gamma_k\to 0$. If the a_j are known for $j>3N$, then we may solve (2.16) using successive consecutive blocks of $3N$ coefficients and hence obtain sequences of estimates for each of the parameters.

The γ_i and y_i dependence in (2.10) is nonlinear; so we must resort to an iterative numerical-solution procedure. The problem is most easily cast in the form of a minimization problem, i.e., to find the point for which

$$\mathfrak{s}(A_i,y_i,\gamma_i)\equiv\sum_{j=J}^{J+3N-1}\left(a_j-\sum_{i=1}^{N}A_i\frac{1}{\gamma_i}\binom{-\gamma_i}{j}(-y_i)^j\right)^2$$

$$\equiv\sum_{j=J}^{J+3N-1}S_j^2\to 0\,. \tag{2.19}$$

There are many numerical procedures available for the minimization of a nonlinear function of several variables including modified Newton–Raphson procedures, gradient procedures, and eigenvector procedures; all of these procedures require starting values for each of the parameters, the required accuracy of which depends upon the nature of the function. However, we have found that for (2.19), even in controlled situations where the starting values are known to be very accurate and for N values as low as 2, the function $\mathfrak{s}$ is so poorly behaved that the repeated application of any one recognized procedure often does not lead to a solution. To solve (2.19) we have developed a diverse strategy method which includes several possible minimization techniques. The first is a modified Newton–Raphson procedure where the step direction $\Delta\vec{\mu}$ is calculated by

$$\sum_{j=1}^{3N}\frac{\partial^2\mathfrak{s}}{\partial\mu_i^*\,\partial\mu_j}\Delta\mu_j=\frac{-\partial\mathfrak{s}}{\partial\mu_i^*}\,, \tag{2.20}$$

and where

$$\mu_i = A_i\ , \quad \mu_{i+N} = \gamma_i\ , \quad \mu_{i+2N} = y_i\ , \quad i = 1, \ldots, N\ . \tag{2.21}$$

Since we deal with series with real coefficients, the singularities are either real or occur in complex-conjugate pairs. In the former case, $\mu_i^* \equiv \mu_i$. In the latter case, the complex-conjugate pair μ_i and μ_{i+1} are relabeled μ_i and μ_i^* for clarity. Two variations of this method where the minimization is performed with respect to the A and γ variables and with respect to the A variables alone respectively, are also used. The other two techniques are a second-order gradient procedure where the step is along the curve, expressed paramatically in t as

$$\Delta\mu_i = \frac{-\partial s}{\partial \mu_i^*}\, t + \frac{1}{2}\sum_j \frac{\partial^2 s}{\partial \mu_i\, \partial \mu_j}\, \frac{\partial s}{\partial \mu_j^*}\, t^2\ , \tag{2.22}$$

and, finally, an "eigenvector" procedure where the step direction is along the eigenvector corresponding to the minimum eigenvalue of the matrix with elements $\partial^2 s/\partial\mu_i^*\,\partial\mu_j$. The local nature of the second-derivative matrix is used to order the procedures according to their likelihood of achieving the greatest reduction in s. The procedures are then attempted in that order, with searches for the minimum along each step direction, until one is found which achieves a sufficient reduction to satisfy a predetermined criterion and that step is taken. If none satisfies our criterion, the one coming closest is used. The diverse strategy approach sacrifices computation time in order to ensure that the best reduction is obtained at each step. Details of this procedure have been published elsewhere.[5]

The use of this basic diverse strategy has enabled us to solve (2.19) for various test functions and for several series from the theory of critical phenomena. However, to improve the efficiency it has been desirable to supplement the features of the basic strategy. In many cases it is possible to use the best estimates obtained from Padé-approximant analysis as starting values of the parameters. However, when reliable estimates of all parameters but the amplitudes are available, it is easy to perform a minimization with respect to the A_i alone, since s is purely quadratic in them. We have also developed a modification of the γ-renormalization procedure, which enables us to obtain reliable starting values for the y_i when the assumption that $\gamma_i = \gamma$ for all i is reasonable and an estimate of γ is available. However, since we are trying to fit $3N$ coefficients (a_j) simultaneously and the freedom to choose the A_i's allows us to fix N of them, the Padé denominator, from the roots of which the y_i's are calculated, is obtained by a "least-squares" matching of $2N$ series terms rather than an exact matching of N terms.

A further optional feature used in conjunction with the diverse strategy is the so-called Davidenko method[6] by which a problem with a known solution is continuously distorted into the one for which the solution is sought. Let us suppose that $\hat{A}_i$, $\hat{y}_i$, and $\hat{\gamma}_i$ are initial estimates of the parameters we seek. We define

$$\hat{a}_j \equiv (\hat{A}_i/\hat{\gamma}_i)\binom{\hat{\gamma}_i}{j}(-\hat{y}_i)^j\ , \tag{2.23}$$

so that $\hat{A}_i$, $\hat{y}_i$, and $\hat{\gamma}_i$ define the minimum point of (2.19) when a_j is replaced by $\hat{a}_j$. The Davidenko problem in this case is to minimize (locate zeros of)

$$s(A_i, y_i, \gamma_i, \lambda) = \sum_{j=J}^{J+3N-1} \left(\hat{a}_j + \lambda(a_j - \hat{a}_j) - \sum_{i=1}^{N} A_i\, \frac{1}{\gamma_i}\binom{\gamma_i}{j}(-y_i)^j\right)^2\ , \tag{2.24}$$

where, for $\lambda = 1$, (2.24) corresponds to (2.19). The standard procedure is to vary λ from 0 to 1 using the solution $A_i(\lambda_k)$, $y_i(\lambda_k)$, $\gamma_i(\lambda_k)$ as the starting point in seeking the solution for λ_{k+1}. Using the identification (2.21), we note that for any solution $s = 0$, the conditions

$$\left.\frac{\partial s}{\partial \mu_j^*}\right|_{\lambda=0} = 0 \tag{2.25}$$

determine the μ_j implicitly as functions of λ. Therefore on the locus of solutions $(\nabla s = 0)$ the condition

$$\sum_{j=1}^{3N} \left.\frac{\partial^2 s}{\partial \mu_j^*\, \partial \mu_i}\right|_{\lambda} d\mu_i + \frac{\partial^2 s}{\partial \mu_j^*\, \partial \lambda}\, d\lambda = 0 \tag{2.26}$$

enables us to calculate $d\mu_i/d\lambda$. Hence we can project even better starting values

$$\hat{\mu}_j(\lambda_{k+1}) = \mu_j(\lambda_k) + \frac{d\mu_j}{d\lambda}\,\Delta\lambda_k\ , \tag{2.27}$$

where $\lambda_{k+1} = \lambda_k + \Delta\lambda_k$ and $\Delta\lambda_k$ is not too large, given the present solution $\mu_j(\lambda_k)$. It is better to make the projections (2.27) on a Riemann sphere rather than in the plane because A_i may pass through infinity as the corresponding γ_i takes positive integer values; and similarly as y_i passes through zero, γ_i passes through infinity, changing signs in the process. The choice of $\Delta\lambda_k$ is arbitrary but we seek to choose it small enough to require only a few iterations to reach the new solution $\mu_j(\lambda_{k+1})$ but large enough not to require too many increments in λ to reach $\lambda = 1$.

D. Extended Form of General Analysis

In order to approximately account for the possibility of a more general form than (1.1) (e.g., additive entire functions, more than N singularities, or variations in the nature of the singularities), we have extended the general form of analy-

sis to match the first $3N+M+D+1$ terms of the series to the form

$$F(x)=\sum_{i=1}^{N}\frac{A_i}{\gamma_i}\left[(1-y_ix)^{-\gamma_i}-1\right]+\frac{P_M(x)}{Q_D(x)}\ , \qquad (2.28)$$

where

$$P_M(x)=\sum_{l=0}^{M}\mathcal{P}_{M-l}x^l$$

and

$$Q_D(x)=\sum_{k=0}^{D}\mathcal{Q}_{D-k}x^k\ . \qquad (2.29)$$

Without loss of generality we may choose the constant coefficient $\mathcal{Q}_D=1$. The second term has the same form as a Padé approximant and it is capable of approximating up to D singularities (admittedly not precisely if they are not simple poles). The inclusion of this term may account for several singularities of lesser importance and mean that reliable approximations can be obtained for smaller N than would be otherwise required.

For $D=0$, $Q_D(x)\equiv 1.0$, Eq. (2.28) has the same form as (2.17) when Eqs. (2.16) are solved for $J=M+1$. The sequences of estimates obtained using the original procedure correspond to the estimates we would obtain fitting (2.28) to the first $3N+M$ terms of the series with $D=0$ and M ranging from 1 to the maximum permitted by the length of the series.

Although we may now do well with a smaller N, for a given N and $D>0$ the problem of solving for the unknown parameters in (2.28) is obviously more difficult. The condition we impose is

$$\sum_{j=0}^{\infty}a_jx^j-\sum_{i=1}^{N}\frac{A_i}{\gamma_i}\left[(1-y_ix)^{-\gamma_i}-1\right]-\frac{P_M(x)}{Q_D(x)}=O(x^{3N+M+D+1})\ . \qquad (2.30)$$

Multiplying (2.30) by $Q_D(x)$ and expanding the functions on the left-hand side, we get

$$\sum_{j=0}^{\infty}\left[\sum_{k=0}^{\min(j,D)}\left(a_{j-k}-\sum_{i=1}^{N}A_i\Gamma_{i,j-k}(-y_i)^{j-k}\right)\mathcal{Q}_{D-k}\right]x^j+\sum_{l=0}^{M}\mathcal{P}_{M-l}x^l=O(x^{3N+M+D+1})\ , \qquad (2.31)$$

where the symbol $\Gamma_{i,m}\equiv(1/\gamma_i)\binom{-\gamma_i}{m}$ for $i\geq 1$, and $\Gamma_{i,0}\equiv 0$. The second term on the left-hand side does not affect powers of x higher than M; so if we select the values of the A_i, γ_i, y_i, and $\mathcal{Q}_{D-k}$ so that the coefficients of x from order $M+1$ to $M+D+3N$ inclusive vanish, then the coefficients $\mathcal{P}_{M-l}$ may later be chosen to satisfy the conditions on the terms from order 0 to M. For this case then we have to solve the nonlinear equations

$$\sum_{k=0}^{\min(j,D)}\left(a_{j-k}-\sum_{i=1}^{N}A_i\Gamma_{i,j-k}(-y_i)^{j-k}\right)\mathcal{Q}_{D-k}=0\ ,$$

$$\mathcal{Q}_D=1\ ,\quad j=M+1,\ M+2,\ \ldots,\ M+D+3N \qquad (2.32)$$

from which we obtain the minimization problem

$$\$=\sum_{j=M+1}^{M+D+3N}\left[\sum_{k=0}^{\min(j,D)}\left(a_{j-k}-\sum_{i=1}^{N}A_i\Gamma_{i,j-k}(-y_i)^{j-k}\right)\mathcal{Q}_{D-k}\right]^2\rightarrow\text{minimum}=0\ , \qquad (2.33)$$

which is the analog of (2.19) for the generalized case.

Rather than minimize \$ simultaneously with respect to the μ's and the $\mathcal{Q}$'s [μ's defined as in (2.21)], we take advantage of the fact that with respect to the $\mathcal{Q}$'s alone Eqs. (2.32) are linear. Our procedure is to choose starting values for the μ's, solve for the $\mathcal{Q}$'s which minimize \$ keeping the μ's fixed, then calculate an increment in the μ's (using the diverse strategy procedure already described) which will tend to minimize \$ with respect to the μ's. The $\mathcal{Q}$'s vary implicitly with the μ's. Since each evaluation of \$ now requires the solution of D linear equations, the computation time rises rapidly with D.

Using this minimization procedure, we have been quite successful in obtaining solutions for small values of D. However, for larger values of D we often encounter difficulty.

III. NUMERICAL RESULTS ON TEST FUNCTIONS

In this section we apply the new methods of analysis to various test functions including the functions labeled $A-K$ from I (where they were analyzed using the previously available procedures). For convenience we list again in Table I the functions

TABLE I. Test functions A–O which we have used to study the effectiveness of the methods of series analysis. Functions A–K are discussed in more detail in Ref. 1.

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	$(1-x)^{-1.5}+(1+\frac{4}{5}x)^{-1.25}+e^{-x}$
L	$(1-x)^{-7/4}+(1-x)^{-1}+(1-x)^{-1/4}+(1-x)^{+1/2}+(1-x)^{+5/4}+e^{-x}$
M	$\frac{\tan x^{1/2}}{x^{1/2}}=\frac{8}{\pi^2}\left(1-\frac{4}{\pi^2}x\right)^{-1}+\frac{2}{\pi^2}+\left(\frac{3}{2\pi^2}-\frac{1}{6}\right)\left(1-\frac{4}{\pi^2}x\right)+\cdots$
N	$(1-x)^{1/2}\,[1+k(1-x)^{1/2}]^{-1}$
O	$\{(1-x)^{1/2}[1+k(1-x)^{1/2}]\}^{-1}$

TABLE II. Location of poles in some Padé approximants.

Poles in [5/6]	Poles in [9/10]	Expected poles
+1.7581	+1.7510	+1.7500
−0.0044 ± 1.9862i	0.0022 ± 2.0033i	± 2.0000i
−0.9939	−0.9968	cut beginning at −1.0000
−1.1106	−1.0460	
−6.3013	−1.2344	
	etc.	

A–K together with the additional test functions we will use in this section.

A. Exponent-Renormalization Method

When this procedure is applied to functions with the precise form (2.1), the $[N-1/N]$ Padé approximant in theory should exactly reproduce the renormalized function, and attempts to calculate $[n+p/n]$, $n>N$, $p\geq -1$, should produce singular matrices. However, numerical roundoff effects which may arise can cause slight deviations from the exact result. Padé approximants $[m/n]$, where $n<N$, are unlikely to give very accurate predictions for the location of n of the poles in the renormalized function unless the $N-n$ other poles are relatively very weak (much further away from the origin or with much smaller amplitude). For example, a Padé approximant forced to approximate two poles of equal amplitude at $x_1=+1$ and $x_2=+2$ by a single pole might have that pole located at $x_{\text{eff}}=1.20$; as x_2 increases or the amplitude of that pole decreases, x_{eff} would move closer to x_1.

If the function being analyzed has the form of (2.1) with an additive entire function as well, the renormalization goes through as before except that now there are contributions from the extra term added to the coefficients. Since the exponent-renormalization transformation carries any entire function into another entire function ($\gamma\neq$ negative integer) the analysis is the same as for a meromorphic function with only a finite number of poles. For $\gamma\approx 1$, $\binom{-\gamma}{n}(-1)^n$ is a slowly varying function of n. We are not surprised, for example, to find that the direct Padé analysis of

$$\mathfrak{F}(x)=\sum_{i=1}^{4}(1-y_i x)^{-1.0}+e^{-3x} \tag{3.1}$$

is qualitatively similar to the Padé analysis of the renormalized function obtained from

$$f(x)=\sum_{i=1}^{4}(1-y_i x)^{-1.5}+e^{+3x}\,, \tag{3.2}$$

where $y_i=-1,\ -\frac{1}{2},\ +\frac{1}{2},\ +1$ for $i=1,\ 2,\ 3,\ 4$.

We have analyzed functions A–K by the method of Sec. II A, renormalizing with respect to three exponent values $\gamma_r=1.25$, $\gamma_r=1.375$, and $\gamma_r=1.5$. For $\gamma_r\neq 1.5$, the dominant singularity at $x=+1$ in each of these functions appears in the Padé approximant to the renormalized function as the beginning of a cut represented by a sequence of poles and zeros beginning near $x=-1.0$ and stretching out along the negative real axis, provided the order of the approximant is sufficiently large. If we denote by $\mathfrak{F}_{Z,\gamma_r}$ the function obtained from a function Z by renormalizing with respect to γ_r, the [5/6] and [9/10] Padés to $\mathfrak{F}_{D,1.25}$ have poles at the locations given in Table II. The singularity in D at $+\frac{18}{7}$ does not appear as a pole in the Padé approximant at $-\frac{18}{7}$, since it would lie on the cut axis. On the other hand, in Padé approximants to $\mathfrak{F}_{D,1.5}$ we would expect to see a pole at $+1.00$ and cuts along all four semiaxes starting at $+\frac{7}{4}$, $-\frac{16}{7}$, and $\pm 2i$. This behavior is approximately what we observe in, say, the [9/10] Padé approximant, although some of the complex poles do not quite fall on the imaginary axes. For E and F using $\gamma_r=1.25$, the behavior we see is similar to that for D, since $x=-1.0$ is already a branch point in $\mathfrak{F}_{D,1.25}$. In $\mathfrak{F}_{F,1.25}$ there is an indication of a cut due to the convergent singularity in F, since it lies opposite the dominant branch point. Using $\gamma_r=1.50$ to renormalize E and F still leaves a cut on the negative real axis, this time caused by the factors multiplying the dominant singularity. Hence there is little difference between $\mathfrak{F}_{E,1.25}$ and $\mathfrak{F}_{E,1.5}$ unless we can form high-enough-order Padé approximants to see the cuts on the other three semiaxes in $\mathfrak{F}_{E,1.5}$.

The behavior of G–I when analyzed by the method of exponent renormalization is as we would expect except that cuts along the line $\mathrm{Re}(x)=1$ are hard to detect since it is already crowded with singularities. The cut on the real axis when $\gamma_r=1.25$ is very apparent in the Padé approximants; it is not so apparent in H and I for $\gamma_r=1.50$.

For J and K the results of this analysis are straightforward: The singularity whose exponent matches the value used for renormalization is represented by the Padé approximant to a very high degree of accuracy; there is a long line of poles and zeros stretching outward from the other singular point.

When the functions are renormalized using $\gamma_r=1.375$ none of the singularities transforms to a simple pole, so that Padé-type approximations to branch cuts abound.

The accuracy with which the exponent-renormalization method predicts the locations of the singularities in the functions A–K is tabulated in Table III for two values of the renormalization exponent, $\gamma_r=1.50$ and $\gamma_r=1.25$. The parameter tabulated is ϵ_n defined in I as

$$\epsilon_n=-\log_{10}\rho_n\,, \tag{3.3}$$

where ρ_n is the relative error in estimating one of

TABLE III. Values of ϵ_n for estimates of y_i using n terms of the series (for functions A–K) by the exponent-renormalization method. Renormalization is performed with respect to two different values: $\gamma_r = 1.50$ (true exponent for $i=1$) and $\gamma_r = 1.25$ (true exponent for $i \geq 2$).

Test		$\gamma_r = 1.50$			$\gamma_r = 1.25$		
series	i	$n=10$	$n=15$	$n=20$	$n=10$	$n=15$	$n=20$
A	1	7.0	>7.0	>7.0	1.8	2.1	2.5
B	1	2.5	3.5	4.0	1.5	2.2	2.4
C	1	2.3	3.1	3.7	1.6	2.2	2.6
D	1	3.1	4.7	7.0	1.4	2.0	2.5
	2	1.2	1.2	2.0	1.6	2.7	3.2
	3,4	1.1	1.4	1.8	1.1	2.1	2.7
	5	•••	•••	•••	•••	•••	•••
E	1	1.9	3.2	4.0	1.7	2.1	2.2
	2	1.1	1.7	1.7	2.3	2.6	2.9
	3,4	0.9	1.4	1.8	1.5	2.2	2.7
	5	•••	•••	•••	•••	•••	•••
F	1	1.9	2.7	3.1	1.7	2.3	2.3
	2	1.1	1.2	1.8	2.0	2.2	3.2
	3,4	0.7	1.4	1.5	1.4	2.4	2.7
	5	•••	•••	•••	•••	•••	•••
G	1	2.4	3.3	4.5	1.5	1.8	2.1
	2,3	•••	1.3	1.7	•••	0.7	2.0
	4,5	•••	1.3	1.5	•••	1.0	2.1
	6,7	•••	0.9	1.2	•••	0.8	1.7
H	1	2.2	2.7	3.2	1.5	1.8	2.0
	2,3	•••	0.5	1.7	•••	0.4	1.4
	4,5	•••	•••	1.4	•••	•••	1.6
	6,7	•••	•••	0.7	•••	•••	0.6
I	1	2.0	2.2	2.4	1.6	1.9	2.1
	2,3	•••	1.5	2.0	•••	1.3	2.7
	4,5	•••	1.4	1.5	•••	1.6	2.1
	6,7	•••	1.0	1.4	•••	1.2	1.7
J	1	6.7	>7.0	>7.0	2.0	2.0	2.6
	2	1.9	2.2	2.5	5.7	>7.0	>7.0
K	1	5.2	>7.0	>7.0	1.8	2.1	2.5
	2	1.6	2.0	2.4	2.6	5.3	>7.0

the critical parameters (in this case y_i) using n terms of the series expansion.

B. Confluent-Singularity Method

As with the first method, when the series being analyzed represents a function which is exactly of the assumed form, in this case (2.4) for finite N, then the $[N-1/N]$ Padé approximant will exactly represent the transformed function. Minor exceptions to this are observed due to rounding effects when the inverses of two exponents are very close together. If $\gamma_N = 0$, i.e., the last term in the function is an additive constant, the transformed function will be exactly represented by the diagonal Padé approximant $[N-1/N-1]$ rather than by $[N-1/N]$.

When an entire function is added to the form (2.4) as in the case of function L (Table I), the transformed function will contain poles corresponding to the leading terms of the Taylor-series expansion of the entire function. These poles tend, with rapidly decreasing residue, to a limit point at $\xi = 0$. Whereas when the last term in L is missing we obtain the five indices exactly from the [4/5] Padé approximant, from the [9/10] Padé approximant to the transform of L we see poles as given in Table IV. The two strongest singularities, corresponding to $\gamma_1 = \frac{7}{4}$ and $\gamma_2 = 1$, are represented accurately. Beyond that the representation of the singularities is much less accurate. There is as expected an infinite sequence of singularities converging on the origin from the expansion of the entire function; the amplitude of these singularities tends to zero as predicted. Hence the Padé approximant shows poles which are compromise values for the more important terms in the Taylor expansion (marked *) and the other three singular terms in the function, but from which, in this order, it is impossible to deduce reasonable values for γ_3, γ_4, and γ_5.

As another example, we have considered the function M whose divergence at the singular point $x = \frac{1}{4}\pi^2$ is described by the expansion which is also given in Table I. The transformed function for M has the form

$$\mathfrak{F}_M(\xi) = A_{+1}(1-\xi)^{-1} + A_0 + A_{-1}(1+\xi)^{-1} + \cdots , \quad (3.4)$$

where $A_{+1} = 0.8106$, $A_0 = 0.2026$, and $A_{-1} = -0.0147$. From the [4/4] Padé approximant we find poles at $\xi_{+1} = 1.0000$ and $\xi_{-1} = -1.1638$, from whose residues we predict $A_{+1} \approx 0.8104$ and $A_{-1} \approx -0.0155$. From an $[n/n]$ Padé approximant we estimate

$$A_0 \approx \lim[n/n] \text{ as } \xi \to \infty , \quad (3.5)$$

and for the [4/4] we obtain $A_0 \approx 0.2034$. {Note: An $[n-1/n]$ Padé approximant will approximate a constant by putting a pole ξ_0 far from the origin so that $A_0(1-\xi/\xi_0)^{-1} \approx A_0$. This was illustrated in the [9/10] Padé approximant in the previous example.} Higher-order Padé approximants show improved

TABLE IV. Padé-approximant poles for the confluent-singularity-method transformation of L.

Expected poles	+0.57	+1	+4	∞^*	−2	-1^*	$-\frac{4}{5}$	$-\frac{1}{2}^*$	$-\frac{1}{3}^*$	$-\frac{1}{4}^*$	$-\frac{1}{5}^*$
[9/10] poles	+0.57	+1.02	+10.50		−1.11	−0.56	−0.30	−0.20	−0.15	−0.11	−0.08

precision in ξ_{-1} and A_{-1} and also approximate additional terms in (3.4).

The function N illustrates a problem which may arise. We expect to see confluence of the form

$$F_N(x) = (1-x)^{1/2} - k(1-x) + k^2(1-x)^{3/2} - k^3(1-x)^2 + \cdots . \quad (3.6)$$

However, for the case $k=1$ (and similarly $k=-1$), the function is singular on one of its branches for $x=0$, i.e., when $(1-x)^{1/2} = -1$. In these special cases, $F_N(x)$ does not have a Taylor-series representation. For $k=\frac{1}{4}$ this singularity moves to $x=-15$. On applying the transformation we see clear estimates for the first two terms in (3.6); for example, from [9/10], $\gamma_1 = -0.500006$, $A_1 = 1.0001$ and $\gamma_2 = -0.9964$, $A_2 = -0.2438$. The other singularities seem to be tending toward their limiting location from off the real axis. For $k = -\frac{1}{4}$ we see the first three terms in (3.6) with accuracy comparable with the above and we note that the remaining roots of the Padé approximant are real. For the test function O, where the confluence we are looking for has the form

$$F_O(x) = (1-x)^{-1/2} - k + k^2(1-x)^{1/2} - k^3(1-x) + \cdots ,$$

the results obtained are qualitatively similar and of about the same accuracy as for N. However, now, because of the constant term, we prefer to look at $[n/n]$ Padé approximants and estimate the constant using (3.5).

The usual Padé-approximant procedures applied to the logarithmic derivatives $[d \ln F(x)/dx]$ of these functions are only capable of revealing the leading exponent at any of these singular points. The estimates obtained by the usual Padé-approximant procedures for N and O are much less accurate; typical values of $\gamma_1 \approx -0.503$, $A_1 \approx 1.02$ are fully two to three significant figures worse than those quoted above for the confluent-singularity method.

We have analyzed test functions A–F using the confluent-singularity method, performing the transformation with $y=1$. Hence we are looking for "confluence" at the location of the strongest singularity. We would expect to see the leading exponent $\gamma_1 = 1.5$ in all six cases. Since A and D have no factor multiplying this singularity, we will see only the effect of an additive Taylor series (since in both cases the additive terms are analytic at $x=1$); that is, subsequent γ's should be 0, -1.0, -2.0, ... However, for B, C, E, and F the dominant singularity is multiplied by a factor analytic at $x=1$, and hence we should also see exponents $+0.5$, -0.5, -1.5, ... in addition to all of the above. The behavior of A is as expected; we are able to see clearly the first six terms from the [9/9] approximant. The leading exponent is given to eight-figure accuracy, the second term (the constant) corresponding to $\gamma=0$ is obtained to five-figure accuracy from (3.5), and the sixth term ($\gamma=-4.0$) is given to 7% accuracy. The behavior of B and C is clearly not the same as for A. The value $\gamma=+0.5$ is clear, while the exponents of the opposite sign are not so distinct and not all the expected values appear. Rather, for B, where the multiplying factor at $x=1$ is three times as great as it is for C, the exponents tend to be closer to the sequence -0.5, -1.5, -2.5, ..., and for C they tend to be closer to the sequence -1.0, -2.0, -3.0, ... The complexity of the functions D–F precludes obtaining any detailed results using this method. For D we do see both the leading singularity to four figures and the constant to two figures. For E and F we obtain the leading γ to two figures, but we can conclude nothing beyond that except that their behavior is not similar to D.

C. General Method

We will denote a generalized approximant of the form (2.28) by the symbol $[N, D, M]$. We have formed such approximants to the series expansions of the functions A–K for various values of N, D, and M and using up to 20 terms of the expansions, i.e., $3N+D+M \leq 19$. As we pointed out earlier, we encounter difficulty in calculating the approximant for other than quite small values of D. We have obtained some approximants with $N=5$ for function D, but these also are difficult to obtain; so usually we rely on the Padé-approximant term to approximate the less important singularities as simple poles. Approximants of the form $[N, 0, M]$ correspond to the procedure described in Sec. II C and, of course, in the new notation $[0, D, M]$ is the usual $[M/D]$ Padé approximant.

The class of approximants for which we have calculated the largest number has the form $[1, D, M]$. The estimates for the parameters describing the strongest singularity which are obtained from such approximants are summarized in Table V. The number tabulated for each value of D is $\epsilon_{3+D+M_{\max}}$. The maximum order of the numerator, $M_{\max}$, may be determined from the column headed "M values" which lists those values of M which we were able to calculate approximants for the given D value. In some cases $M_{\max}$ is not the maximum value which is theoretically possible given 20 terms of the series.

In considering the pattern of divergent singularities in the functions A–K, the functions obviously fall into four groups: three groups of three in consecutive order with J and K forming the fourth group. We note that J is exactly of the form (2.1), A, D, G, and K are close to that form, and the remaining functions differ more from that form in that the strongest singularity is multiplied by some function of x. However, in Table V we are

TABLE V. Values of ϵ_{20} for estimates of y_1 and γ_1 from $(1, D, M)$ generalized approximants to the functions A–K. The value tabulated for each value of D represents the best estimate from a sequence of approximants for the various M values shown in the last column.

Series	D	y_1	γ_1	M values
A	0	>10	>10	1–16
	1	>10	>10	0–15
	2	>10	8.4	1–14
	3	>10	8.4	2–13
	4	>10	8.4	3–12
	5	9.0	7.7	6–7
B	0	3.1	1.7	1–16
	1	3.5	1.9	0–15
	2	3.0	1.7	1–3, 5–7
	3	3.0	1.7	2–6
C	0	2.7	1.3	3–16
	1	3.1	1.5	0–15
	2	2.8	1.3	1–4, 6–9
D	0	3.1	2.0	0, 1, 4–16
	1	4.0	3.0	0–15
	2	4.0	3.0	1–3, 5–7, 9–11, 13, 14
	3	5.2	4.2	2–9, 11–13
	4	5.4	4.3	3–6, 8–12
	5	4.9	3.8	5–8
	6	4.2	3.3	5
E	0	2.9	1.6	0–16
	1	3.1	1.7	1–15
	2	3.0	1.6	1–3, 5–7, 9, 11, 12
	3	2.9	1.6	2–11
F	0	2.2	1.5	4, 6, 8–16
	1	2.6	1.3	0–15
	2	2.6	1.3	1–3, 5–7, 9, 10, 12, 14
	3	2.5	1.2	2–12
	4	2.9	1.4	3–8, 10–12
G	0	1.9	0.9	0–12, 16
	1	1.5	0.6	0–2, 4, 5, 7, 8
	2	2.3	1.2	1, 3–5, 7–9
	3	1.7	0.8	2–4
H	0	2.2	1.3	0–16
	1	2.5	1.3	0–2, 4, 5
	2	2.5	1.7	1, 3–12
	3	2.5	1.3	2, 3
I	0	1.6	0.4	1–11
	1	1.1	0.2	0–2, 4, 5, 7, 8
J	1	3.8	2.7	0–15
	2	6.5	5.5	1–9, 12–14
	3	7.2	6.3	2, 5, 8
K	1	3.8	2.7	0–15
	2	6.5	5.5	1–4, 7–14
	3	3.6	2.9	3, 4

considering only approximants with $N=1$; so none of the functions will be exactly representable by such an approximant. Function A is most closely representable by (2.28) with $N=1$, since e^{-x} is entire and the coefficients in its expansion drop off as $(n!)^{-1}$ and are therefore well represented by a low-order Padé approximant. The estimates obtained for A in Table V are very close to the true value. The estimates for D are considerably better than those for E and F, reflecting the compatibility of the form of D. Similarly, one might expect G to be more amenable to this analysis than H or I, but Table V shows this is not the case. However, in G–I the second and third singularities are only about 10% further from the origin than the first one, and approximating these strong algebraic singularities by simple poles introduces a considerable error into the $[1, D, M]$ approximants. In fact, we note that the estimates of y_1 and γ_1 are more accurate for H where A_1, the effective amplitude of the closest singularity, is larger than for G and I. The functions J and K both have two singularities of approximately equal strength on opposite sides of the origin. Any attempt to approximate these functions by an approximant containing only one singularity is unrewarding. Therefore

TABLE VI. Comparison of accuracy of estimates (tabulation of ϵ_{20}) of the locations y_i of the singularities in functions A–K using the $[1, D, M]$ generalized approximants, and the ordinary Padé approximants $[M/D] \equiv [0, D, M]$ to the logarithmic derivatives of the functions.

Test series	i	Exact location of singularity y_i	ϵ_{20} for generalized-approximant analysis	ϵ_{20} for usual Padé approximant analysis
A	1	1.0000	>10	4.8
B	1	1.0000	3.5	5.1
C	1	1.0000	3.1	4.0
D	1	1.0000	5.4	3.5
	2	−1.7500	1.7	2.2
	3, 4	$\pm 2.0000i$	1.7	2.0
	5	2.2857	1.1	•••
E	1	1.0000	3.8	3.7
	2	−1.7500	1.4	2.2
	3, 4	$\pm 2.0000i$	0.7	1.8
	5	2.2857	•••	•••
F	1	1.0000	2.9	2.7
	2	1.7500	1.6	2.1
	3, 4	$\pm 2.0000i$	1.5	2.0
	5	2.2857	•••	•••
G	1	1.0000	2.3	2.7
	2, 3	$1.0000 \pm 0.4816i$	0.5	0.9
	4, 5	$1.0000 \pm 1.2540i$	•••	0.5
	6, 7	$1.0000 \pm 4.3813i$	•••	0.5
H	1	1.0000	2.5	2.4
	2, 3	$1.0000 \pm 0.4816i$	0.6	0.9
	4, 5	$1.0000 \pm 1.2540i$	•••	0.5
	6, 7	$1.0000 \pm 4.3813i$	•••	0.2
I	1	1.0000	1.6	2.2
	2, 3	$1.0000 \pm 0.4816i$	•••	1.0
	4, 5	$1.0000 \pm 1.2540i$	•••	1.0
	6, 7	$1.0000 \pm 4.3813i$	•••	0.7
J	1	1.0000	7.2	4.4
	2	−1.2500	2.0	4.2
K	1	1.0000	6.5	3.9
	2	−1.2500	2.1	2.7

TABLE VII. Estimates for y_i, γ_i, $A_i\gamma_i$, $i=1,2$, for the function K using $[2,D,M]$ generalized approximants.

M	$D=0$	$D=1$	$D=0$	$D=1$	$D=0$	$D=1$
	y_1		γ_1		$A_1\gamma_1$	
0	1.053 302 075	1.021 118 441	1.235 295 184	1.382 732 649	1.558 321 056	1.535 267 203
1	1.005 551 024	0.980 876 269	1.473 025 520	1.639 848 163	1.501 437 690	1.421 497 617
2	0.988 715 721	0.998 395 175	1.578 433 014	1.511 953 108	1.459 429 408	1.492 432 677
3	1.004 489 791	1.000 251 649	1.464 432 204	1.497 837 613	1.526 520 128	1.501 802 732
4	0.998 862 991	0.999 962 931	1.510 241 807	1.500 359 342	1.490 855 267	1.499 641 862
5	1.000 220 611	1.000 004 899	1.497 789 382	1.499 947 284	1.502 312 014	1.500 060 123
6	0.999 964 678	0.999 999 422	1.500 390 002	1.500 006 824	1.499 540 946	1.499 991 338
7	1.000 004 840	1.000 000 061	1.499 941 654	1.499 999 214	1.500 075 779	1.500 001 090
8	0.999 999 419	0.999 999 994	1.500 007 590	1.500 000 082	1.499 989 293	1.499 999 878
9	1.000 000 062	1.000 000 001	1.499 999 126	1.499 999 992	1.500 001 324	1.500 000 012
10	0.999 999 994	1.000 000 000	1.500 000 090	1.500 000 001	1.499 999 854	1.499 999 999
11	1.000 000 001	1.000 000 000	1.499 999 991	1.500 000 000	1.500 000 015	1.500 000 000
12	1.000 000 000	1.000 000 000	1.500 000 001	1.500 000 000	1.499 999 999	1.500 000 000
13	1.000 000 000	•••	1.500 000 000	•••	1.500 000 000	•••
	y_2		γ_2		$A_2\gamma_2$	
0	0.877 532 421	0.904 703 326	0.429 095 856	1.419 282 159	2.440 232 120	0.361 333 356
1	0.973 088 747	0.937 481 957	0.083 056 919	0.231 272 564	2.725 925 743	2.492 997 579
2	0.920 171 195	0.697 984 970	0.328 190 707	2.661 023 675	2.311 931 387	0.536 231 230
3	0.848 583 628	0.789 831 652	0.797 898 999	1.374 971 145	1.689 457 731	1.136 861 412
4	0.814 161 710	0.798 631 567	1.096 607 900	1.267 817 204	1.394 404 959	1.231 964 444
5	0.803 294 100	0.799 812 091	1.209 928 427	1.252 639 170	1.290 027 628	1.246 994 495
6	0.800 643 923	0.799 975 502	1.241 362 181	1.250 371 361	1.259 428 056	1.249 543 420
7	0.800 108 840	0.799 997 028	1.248 406 097	1.250 048 488	1.251 894 605	1.249 936 196
8	0.800 016 215	0.799 999 666	1.249 742 595	1.250 005 841	1.250 330 117	1.249 991 832
9	0.800 002 160	0.799 999 965	1.249 963 048	1.250 000 647	1.250 050 654	1.249 999 044
10	0.800 000 259	0.799 999 996	1.249 995 249	1.250 000 072	1.250 006 908	1.249 999 888
11	0.800 000 028	0.799 999 999	1.249 999 444	1.250 000 011	1.250 000 851	1.249 999 984
12	0.800 000 003	0.800 000 001	1.249 999 947	1.249 999 980	1.250 000 085	1.250 000 033
13	0.800 000 000	•••	1.249 999 992	•••	1.250 000 014	•••

we have omitted the case $D=0$ for $N=1$. The accuracy of the estimation for y_1 and γ_1 is very good for J and K even though the more distant singularity is approximated by a simple pole. The difference between J and K is hardly noticeable, since the e^{-x} term is so insignificant in its contribution to the 20th term.

The last feature of the results in Table V that we emphasize is the marked improvements in estimates for y_1 and γ_1 for function D when the order of the Padé-approximant denominator increases to 3. This at first seems rather odd, since D contains four additional singularities. However, for third-order denominators the Padé-approximant-type term has singularities which approximate the two imaginary and the negative real singularity quite well. The fifth singularity lies well beyond the dominant singularity on the positive real axis. Its contribution to the series coefficients is qualitatively similar to the main contribution, and quantitatively is only a small perturbation to it. Hence it is much less important to the form of the function than the dominant singularity and the other three lesser ones. Once the generalized approximant is able to reproduce these four singularities—one on each axis—the accuracy of the estimates improves by more than an order of magnitude.

In Table VI we compare estimates for the locations of all the singularities obtained from the [1, D, M] generalized approximants and from the standard Padé-approximant analysis of the logarithmic derivative of the function. In the former case the locations of the secondary singularities are estimated from the poles of the Padé-approximant-type term when such estimation is possible. In general, the ordinary Padé-approximant analysis gives better estimates for the location of the secondary singularities, since they are not constrained to be simple poles. One exception to this is the case of the fifth singularity in D, where the generalized approximants yield estimates with $\epsilon = 1.1$, while there is no indication of this singularity in the standard Padé-approximant analysis. Estimation of the dominant singularity in A, D, J, and K [that is, most of the cases that are exactly or nearly of the form (1.1)] is markedly better using the generalized approximants. When the form of the function is altered by multiplying the dominant singu-

TABLE VIII. Estimates for y_i, γ_i, $A_i\gamma_i$, $i=1\ldots5$ for function D using $[5, D, M]$ generalized approximants.

	y_1	y_2	y_5	$\mathrm{Re}y_3=\mathrm{Re}y_4$	$\lvert\mathrm{Im}\,y_3\rvert=\lvert\mathrm{Im}\,y_4\rvert$
(5, 0, 0)	1.000 003 246	0.572 594 498	0.429 669 758	0.000 687 850	0.500 723 412
(5, 0, 1)	0.999 998 082	0.572 420 606	0.448 865 408	0.000 486 788	0.501 932 865
(5, 0, 2)	1.000 001 224	0.572 233 257	0.420 427 151	0.001 020 129	0.501 694 768
(5, 0, 3)	0.999 999 534	0.572 050 476	0.457 261 493	0.000 729 852	0.500 017 867
(5, 0, 4)					
(5, 1, 0)	0.999 998 121	0.572 418 313	0.448 532 828	0.000 468 824	0.501 929 651
(5, 1, 1)	1.000 000 092	0.570 622 244	0.437 166 719	0.000 006 473	0.501 062 620
(5, 1, 2)					
(5, 1, 3)					
exact	1.000 000 000	0.571 428 571	0.437 500 000	0.000 000 000	0.500 000 000
	γ_1	γ_2	γ_5	$\mathrm{Re}\gamma_3=\mathrm{Re}\,\gamma_4$	$\lvert\mathrm{Im}\,\gamma_3\rvert=\lvert\mathrm{Im}\,\gamma_4\rvert$
(5, 0, 0)	1.499 950 790	1.215 409 960	1.300 654 019	1.218 112 693	0.009 827 343
(5, 0, 1)	1.500 030 826	1.218 219 919	1.087 491 525	1.198 067 963	0.009 422 286
(5, 0, 2)	1.499 978 981	1.221 578 540	1.478 706 078	1.198 733 836	0.018 524 353
(5, 0, 3)	1.500 008 568	1.225 182 098	0.902 732 388	1.233 452 808	0.016 763 614
(5, 0, 4)					
(5, 1, 0)	1.500 030 192	1.218 261 086	1.091 744 831	1.198 084 950	0.009 088 721
(5, 1, 1)	1.499 998 362	1.270 200 482	1.225 739 995	1.212 213 952	0.000 060 843
(5, 1, 2)					
(5, 1, 3)					
exact	1.500 000 000	1.250 000 000	1.250 000 000	1.250 000 000	0.000 000 000
	$A_1\gamma_1$	$A_2\gamma_2$	$A_5\gamma_5$	$\mathrm{Re}\,A_3\gamma_3=\mathrm{Re}\,A_4\gamma_4$	$\lvert\mathrm{Im}\,A_3\gamma_3\rvert=\lvert\mathrm{Im}A_4\gamma_4\rvert$
(5, 0, 0)	1.500 079 989	0.648 748 706	0.467 097 852	0.556 797 025	0.002 506 934
(5, 0, 1)	1.499 947 384	0.647 433 816	0.485 565 597	0.563 621 570	0.004 041 014
(5, 0, 2)	1.500 037 834	0.645 650 268	0.427 098 497	0.565 299 830	0.007 413 702
(5, 0, 3)	1.499 983 756	0.643 532 371	0.566 436 864	0.549 330 050	0.008 438 881
(5, 0, 4)					
(5, 1, 0)	1.499 948 491	0.647 411 860	0.484 803 552	0.563 639 473	0.003 904 195
(5, 1, 1)	1.500 003 025	0.604 292 963	0.468 785 426	0.558 927 550	0.005 837 795
(5, 1, 2)					
(5, 1, 3)					
exact	1.500 000 000	0.614 167 635	0.439 852 494	0.525 560 260	0.000 000 000

larity by some function of x, the Padé-approximant estimates are either clearly better (functions B and C) or about the same accuracy (function E, F, H, and I). The relatively poor results for G using the generalized approximants have already been discussed.

We have not completed the analysis for all N values greater than one. For example, to analyze functions G–I with $N=7$ (the number of divergent singularities) would seem beyond the limits of the present method of solution and computer capabilities, judging from present experience. To analyze B and C with $N>1$ would necessitate using N large enough to include several terms in the Taylor-series expansion. These functions are much better suited to analysis by the method for confluent singularities.

The function J is exactly representable by (2.22) with $N=2$ and $P_M(x)\equiv0$ for all M and D. This solution is readily found provided reasonable starting estimates are provided. For K we would expect to get very accurate representations for $N=2$. We have obtained solutions for $D=0$, 1, 2, 3, 4 and we tabulate these for $D=0$ and $D=1$ in Table VII. For $D=2$, 3, 4, the progression toward the exact parameters is even faster, except that the sequences are not complete. The computer program in several instances encounters relative minima in S which prevent it from finding the true solution to the nonlinear equations. Since y_1 and γ_1 are quite close in magnitude to y_2 and γ_2, the apparent convergence of the sequences in Table VII is only slightly faster for the parameters describing the stronger singularity. If one expands the Padé-approximant term, it is obviously very close to the expansion of e^{-x} with the necessary modification to the constant term. For example, for [2, 0, 13] the difference between the tenth term in the expanded Padé-approximant term and 1/10! is only seven parts in 10 000. The approximate relation-

ship $\Delta y/y : \Delta\gamma : \Delta A/A$ as $1 : J : J\ln J$ (where J is the order of last term used) derived in I is evident in Table VII.

Finally, for test function D we have succeeded in obtaining some solutions for $N=5$. This result is the largest value of N for which we have found solutions, and although enough coefficients can easily be calculated to permit solutions with second- and higher-order denominators, the solutions we have found have only been for $D=0$ and $D=1$. The solutions we have obtained are given in Table VIII. The form of D differs from (1.1) in that the "amplitudes" other than A_1 are not constant. The results in Table VIII indicate that the estimates pertaining to the four incorrectly represented singularities are much less precise than those for the first singularity. The instability apparent in the estimates for the fifth (weakest) singularity is further evidence that the form of the function is not as represented and that higher-order denominators in the Padé-approximant-type terms would be necessary for any sort of reasonable representation to be effected.

IV. APPLICATION TO ISING MODEL

A. Exponent-Renormalization Method

We have applied this method to the Ising-model low-temperature-susceptibility expansions in zero field,[7] since one reason for deriving this procedure was the observation that the exponents of the interfering singularities in these functions were quite close to the best estimate for γ'. Padé-approximant analysis of these singularities, whose locations have been given by Domb and Guttmann,[8] indicates that they all have exponents approximately equal to $1\frac{1}{8}$, while γ' is variously estimated[9] between $1\frac{1}{4}$ and $1\frac{5}{16}$. We have analyzed these series by renormalizing with exponent values of 1.1250, 1.1875, 1.2500, 1.3125, and 1.3750. We conclude that the singularities do not share some intermediate exponent value and that little can be added to the conclusions based on ordinary Padé-approximant analysis. When the renormalization exponent is 1.125, the locations of all the interfering singularities are estimated most precisely, while the estimates of the Curie point fluctuate more widely and in some cases appear to be the beginning of a row of poles and zeros along the positive real axis. On the other hand, when the renormalization is performed with respect to values of 1.2500 and 1.3175, the interfering singularities are located much less precisely and the fluctuation in Curie-point estimates is considerably reduced. As far as distinguishing between $\gamma' = 1\frac{1}{4}$ and $\gamma' = 1\frac{5}{16}$ as a preferred value is concerned, the same ambiguity persists as was present in earlier anal-

TABLE IX. Estimates of the high-temperature specific-heat exponent $\alpha = \gamma_1 - j$ from the application of the confluent-singularity method of analysis to jth-order derivatives of the specific-heat series in x. For the fcc lattice, $j=1$ and $x=v$; for the bcc and sc lattices, $j=2$ and $x=v^2$.

fcc lattice						
$D \backslash N$	3	4	5	6	7	8
3	0.154 68	0.108 09	0.129 76	0.112 64	0.167 67	−0.054 12
4	−0.069 17	0.123 37	0.120 77	0.124 68	0.122 81	0.083 21
5	0.115 53	0.120 30	0.122 66	0.123 27	0.124 86	
6	0.120 87	0.111 39	0.123 23	0.122 69		
7	0.128 48	0.124 25	0.117 54			
8	0.121 53	0.130 34				
bcc lattice						
$D \backslash N$	1	2	3	4	5	6
1	0.127 58	0.081 28	0.228 93	−0.017 35	0.113 24	0.857 61
2	0.074 81	0.116 26	0.133 87	0.063 63	−0.040 61	
3	0.263 95	0.132 64	0.121 64	0.121 16		
4	0.246 36	0.086 84	0.121 15			
5		0.157 55				
6	0.441 82					
sc lattice						
$D \backslash N$	1	2	3	4	5	6
1	0.396 18	−0.223 11	0.789 49	−0.134 22		
2	0.191 03	0.107 71	0.207 42		−0.239 36	0.751 45
3	0.092 13	0.147 55	0.124 51	0.118 14	0.119 57	
4	0.221 80	0.120 10	0.116 49	0.119 31		
5	2.087 77	0.116 81	0.118 46			
6		0.120 08				

TABLE X. Estimates of $y_1 = v_c^{-1}$ for the fcc, bcc, sc, and diamond lattices from $[1, D, M]$ generalized approximants to the high-temperature-susceptibility series.

N	$D=0$	$D=1$	$D=2$	$D=3$	$D=4$
fcc					
0	9.909 90	9.834 09	•••	•••	•••
1	9.834 50	9.823 47	9.827 23	•••	•••
2	9.824 80	9.827 28	9.832 51	9.830 06	•••
3	9.828 10	9.838 86	9.830 07	9.830 13	9.819 27[a]
4	9.830 92	9.830 67	9.830 13	9.830 09	9.829 74
5	9.830 64	9.817 37[a]	9.829 75		•••
6	9.830 06	9.829 56	9.829 80	•••	•••
7	9.829 79	9.829 73	•••	•••	•••
8	9.829 74	•••	•••	•••	•••
bcc					
0	7.000 00	5.836 17	•••	•••	
1	6.020 41	6.432 39	6.400 58	•••	
2	6.710 71	6.401 17	6.408 60	6.407 43	
3	6.156 93	6.410 55	6.407 44		
4	6.619 40	6.406 02	6.407 70		
5	6.226 01	6.408 65	6.407 30		
6	6.564 77	6.405 95	6.406 82		
7	6.267 07	6.407 22	6.406 55	•••	
8	6.530 82	6.405 84	•••	•••	
9	6.293 98	•••	•••	•••	
sc					
0	5.000 00	4.245 61	•••	•••	
1	4.360 00	4.630 18	4.591 64	•••	
2	4.813 55	4.592 92	4.579 03	4.580 79	
3	4.390 55	4.582 15	4.580 82		
4	4.736 80	4.580 97	4.581 92		
5	4.455 31	4.585 66	4.584 51		
6	4.696 56	4.584 15	4.584 82		
7	4.486 98	4.585 33	4.584 74	•••	
8	4.671 57	4.584 16	•••	•••	
9	4.506 03	•••	•••	•••	
diamond					
0	3.000 00	3.000 00	•••	•••	•••
1	3.000 00	3.000 00	2.792 25	•••	•••
2	3.000 00			2.793 04	•••
3	2.555 56	2.754 63	2.807 14	2.835 45	2.828 28
4	2.912 80	2.851 60	2.884 91	2.828 79	2.827 28
5	2.839 00	2.869 37	2.856 40	2.827 53	2.825 08
6	2.890 26	2.850 79		2.826 64	2.827 08
7	2.720 19	2.804 32	2.818 33	2.827 51	2.827 20
8	2.886 09	2.830 49	2.848 18	2.827 06	2.827 03
9	2.802 62	2.839 41	2.834 00	2.827 03	
10	2.868 22	2.829 41		2.826 59	•••
11	2.773 46	2.820 17		•••	•••
12	2.865 42	2.826 67	•••	•••	•••
13	2.798 53	•••	•••	•••	•••

[a]The approach to the minimum is extraordinarily slow for these approximants, suggesting a relative minimum rather than a solution.

yses. We consider two criteria for such an assessment, neither of them truly definitive. These are (i) the amount of fluctuation in estimates and (ii) the consistency with predictions of the location of the Curie point from high-temperature-susceptibility series. For the fcc lattice the first criterion favors $\gamma' = 1\frac{5}{16}$ and the second favors the lower value. For the bcc lattice both criteria indicate a marked preference for $\gamma' = 1\frac{1}{4}$, although a value of 1.26 or 1.27 (consistent with Padé-approximant estimates) might be better still. For the sc there is a slight indication from the second criterion that γ' is closer to the larger value, although the fluctuation is about the same for both values of the index. For the diamond lattice there is a strong indication for $1\frac{5}{16}$ using both criteria.

B. Confluent-Singularity Method

We have applied the confluent-singularity method to the spin-$\frac{1}{2}$ Ising-model series for susceptibility and specific heat at both high[10] and low temperatures. We find no evidence that any of the known singularities have weaker singularities confluent with them. However, in the case of the high-temperature specific heat, the results obtained using the transformation are noteworthy for another reason. As indicated previously, the root in the transformed series corresponding to the inverse of an exponent such as α will be hard to detect because of its distance from the origin. However, we have differentiated the series as was suggested by Hunter[11] to reduce the effect of the correction terms, but in this case the differentiation also serves to move the pole closer to the origin. The values of α tabulated in Table IX are calculated from the Padé approximants to the transforms of the second derivative of the fcc specific heat expanded in v and the first derivatives of the bcc and sc specific heats expanded in v^2. We use critical-point values $y = v_c^{-1}$ of 9.8290, 6.4055, and 4.5844[12] for the fcc, bcc, and sc lattices, respectively. The estimates we obtain are in very good agreement with the biased ratio estimates of Sykes *et al.*[3] and hence with the accepted value $\alpha = \frac{1}{8}$. Our analysis using the confluent-singularity transformation is more consistent with $\alpha = \frac{1}{8}$ than is the standard Padé-approximant analysis of the derivatives of the specific-heat series.[11]

In other cases the values indicated for the exponents of the known singularities are all consistent with, and no more precise than, estimates obtained from other methods. We conclude that the poor behavior of the low-temperature series is not attributable to confluent singularities that would have been invisible to other methods of analysis.

C. General Method

We have analyzed series expansions for the Ising zero-field high-temperature susceptibility (HT χ), specific-heat (HT C_H), and low-temperature susceptibility (LT χ) using the method of Sec. II D. For HT χ we have looked at the series for several lattices. For HT C_H we have looked at the fcc expansions since previous analyses indicate most can be learned from the more complete, albeit lower-order, expansion on this lattice. For LT χ we encountered considerable difficulty obtaining solutions for the sc lattice, the lattice for which there is only one interfering singularity; hence we have not attempted the analysis for more difficult situations.

The estimates for y and γ for HT χ are given for

four three-dimensional lattices in Tables X and XI, respectively. The most notable aspect of these results is that the γ estimates are consistently just a little lower than ratio and Padé-approximant results have indicated. Estimates for y are correspondingly slightly higher than the most recent estimates.[12] However, the revised estimates, based on longer series, all represent increases from previously accepted values[13] as compared in Table XII.

The generalized approximants for the diamond lattice undergo a rather marked change as D changes from 2 to 3. The strong oscillation present for $D \leq 2$ disappears, indicating that, in addition to the antiferromagnetic singularity on the negative real axis, there are two other nearby singularities. Closer examination of the standard Padé table indicates a similar onset of stability as the order of the denominator increases from 3 to 4. These other singularities are very roughly at $x = \pm 0.5i$.

Form (2.28) should be very well suited to the HT C_H, since this is essentially the form used by Sykes *et al.*[3] to represent the specific heat for all temperatures above the Curie point. We have calculated most of the generalized approximants for $N=1$, $D \leq 2$ for the fcc specific heat, as shown in Table XIII. Specific-heat series are much more notorious than susceptibility series and, as the results in Table XIII are unbiased in the sense that no estimate depends upon an assumed value for any other parameter, the consistency of these results with ratio results is noteworthy. The deviations in the α estimates, i.e., $\alpha = \frac{2}{15}$, from the accepted value $\alpha = \frac{2}{16}$ are certainly greater than for the ratio sequence calculated by Sykes *et al.* using $\alpha_n = n(a_n/a_{n-1})y^{-1} - n + 1$, where the a_n are the coeffi-

TABLE XI. Estimates of the high-temperature-susceptibility exponent $\gamma_1 = \gamma$ from $[1, D, M]$ generalized approximants.

N	$D=0$	$D=1$	$D=2$	$D=3$	$D=4$
fcc					
0	1.220 18	1.244 78	...	...	...
1	1.244 61	1.249 53	1.247 57	...	...
2	1.248 80	1.247 54	1.244 02	1.245 91	...
3	1.247 03	1.237 50	1.245 90	1.245 86	1.268 37[a]
4	1.245 25	1.245 43	1.245 86	1.245 90	1.246 24
5	1.245 45	1.269 04[a]	1.246 23		...
6	1.245 94	1.246 45	1.246 18	...	...
7	1.246 19	1.246 25	...	...	...
8	1.246 24	...	...	...	...
bcc					
0	1.000 00	1.635 18	...	...	
1	1.488 14	1.226 65	1.248 50	...	
2	1.026 46	1.248 00	1.242 03	1.243 10	
3	1.478 57	1.240 17	1.243 09		
4	1.025 93	1.244 65	1.242 82		
5	1.469 86	1.241 64	1.243 28		
6	1.032 79	1.245 14	1.243 92		
7	1.461 87	1.243 30	1.244 32	...	
8	1.039 37	1.245 51	...	...	
9	1.454 77	...	...	...	
sc					
0	1.000 00	1.564 34	...	...	
1	1.440 37	1.205 01	1.241 51	...	
2	1.021 98	1.240 03	1.257 03	1.254 43	
3	1.505 82	1.252 50	1.254 39		
4	1.030 26	1.254 15	1.252 78		
5	1.474 43	1.246 63	1.248 67		
6	1.039 12	1.249 37	1.248 07		
7	1.461 31	1.246 96	1.248 23	...	
8	1.047 95	1.249 59	...	...	
9	1.453 84	...	...	...	
diamond					
0	1.000 00	1.000 00	...	...	...
1	1.000 00	1.000 00	1.817 98	...	...
2	1.000 00			1.323 99	...
3	1.869 57	1.405 10	1.289 08	1.224 16	1.242 10
4	1.027 04	1.174 18	1.078 85	1.240 68	1.244 99
5	1.209 69	1.127 13	1.162 35	1.244 20	1.253 42
6	1.064 10	1.178 93		1.246 70	1.245 52
7	1.630 80	1.326 69	1.277 16	1.243 94	1.245 08
8	1.019 80	1.229 59	1.153 02	1.245 65	1.245 80
9	1.347 89	1.193 62	1.216 09	1.245 79	
10	1.065 48	1.236 60		1.247 79	...
11	1.511 93	1.279 69		...	...
12	1.046 17	1.246 67	...	...	...
13	1.405 78	...	...	...	...

[a]See Ref. a in Table X.

TABLE XII. Comparison of the best 1967, 1972, and present estimate of v_c^{-1}.

	Old (Ref. 13)	New (Ref. 12)	Present results by general method
fcc	9.8280	9.8290	9.8300
bcc	6.4032	6.4055	6.4065
sc	4.5840	4.5844	4.5847
diamond	2.8262	2.8262[a]	2.8270

[a]Reference 14.

TABLE XIII. Estimates for $y_1 = v_c^{-1}$ and $\gamma_1 = \alpha$ for the high-temperature specific heat from $[1, D, M]$ generalized approximants to the series for the fcc lattice.

M	$D=0$	$D=1$	$D=2$	$D=3$
Estimates for $y_1 = v_c^{-1}$				
2	8.3849	9.9973		
3	8.8564		9.1602	9.8650
4	9.7720		9.8407	9.8725
5	10.0497	9.9751	9.8692	
6	9.9489		9.8130	
7	9.8641	9.8041	9.8192	
8	9.8280	9.8152	9.8227	
9	9.8185		9.8236	...
10	9.8186		...	...
11	9.8206	...	...	...
Estimates for α				
2	0.915 75	−0.132 21		
3	0.654 09		0.557 92	−0.091 39
4	0.124 28		0.111 65	0.085 09
5	−0.044 95	0.005 13	0.088 11	
6	0.025 52		0.143 89	
7	0.094 57	0.154 11	0.136 74	
8	0.127 93	0.141 54	0.132 26	
9	0.137 74		0.130 94	...
10	0.137 65		...	...
11	0.135 12	...	...	...

TABLE XIV. Estimates of y_1, $y_2=u_c^{-1}$, γ_1, $\gamma_2=\gamma'$ from $[2, D, M]$ generalized approximants to the low-temperature-susceptibility expansion on the sc lattice.

$[N, D, M]$	y_1	y_2	γ_1	γ_2
[2, 0, 0]	3.2926	2.3694	1.4948	1.4013
[2, 0, 1]	3.3329	2.2892	1.4317	1.5622
[2, 0, 2]	3.4277	2.5566	1.2615	0.9604
[2, 0, 3]	3.4663	2.4004	1.1839	1.3619
[2, 0, 4]	3.4788	2.4720	1.1554	1.1424
[2, 0, 5]	3.4846	2.4250	1.1406	1.3044
[2, 0, 6]	3.4855	2.4350	1.1381	1.2653
[2, 0, 7]	3.4872	2.4064	1.1326	1.3897
[2, 0, 8]	3.4885	2.4366	1.1282	1.2462
[2, 0, 9]	3.4904	2.3778	1.1215	1.5544
[2, 0, 10]	3.4918	2.4440	1.1158	1.1812
[2, 1, 0]	3.3315	2.2849	1.4343	1.5733
[2, 1, 1]	3.7203	2.3977	0.5503	1.3320
[2, 1, 2]	3.4925	2.4584	1.1196	1.1917
[2, 1, 3]	3.4845	2.4499	1.1402	1.2149
[2, 1, 4]	3.4894	2.4435	1.1260	1.2351
[2, 1, 5]	3.4856	2.4332	1.1377	1.2726
[2, 1, 6]				
[2, 1, 7]	3.4919	2.4212	1.1135	1.3222
[2, 1, 8]				
[2, 1, 9]	3.4966	2.4090	1.0913	1.3825
[2, 2, 1]	3.4814	2.4493	1.1482	1.2159
[2, 2, 2]	3.4837	2.4511	1.1425	1.2112
[2, 2, 3]	3.4871	2.4189	1.1329	1.3537

cients in the expansion. However, the latter sequence is biased, and hence converges faster, since the value of y used comes from HT χ estimates. The estimates of y from our analysis of the specific-heat series are slightly lower than those from the susceptibility series, which is consistent with the slightly higher value of α. Physically, of course, we expect the same location for the singularity from both series.

The incomplete table of generalized approximants for LT χ on the sc lattice is reproduced in Table XIV. We seek approximants with $N=2$ to account for the strong singularity on the negative real axis and the Curie singularity; any other features will hopefully be absorbed in the Padé-approximant term. Estimates of y_1 and γ_1 are consistent with Padé-approximant and exponent-renormalization results. For $D=0$ there is a strong oscillation in γ_2 which appears to be diverging as M increases. This would indicate either that there are other singularities that should be approximated by increasing N or D, or that form (2.28) is not at all reasonable for the LT χ. The oscillation is less pronounced for $D=1$ (and presumably for $D=2$) but there is no indication that even $D=2$ is sufficient to fit (2.28) to the series. We have expended considerable effort in attempts to extend the table using various starting estimates for the parameters and resorting to the Davidenko procedure. If it were possible to solve for higher D values, one might observe the sudden disappearance of the oscillation as was noted in the HT χ for the diamond lattice. There is no hard evidence from standard Padé-approximant analysis of other singularities beyond the physical one, but nevertheless we have tried $N=3$ and used several starting values for the third singularity, placing it confluent with each of the two known singularities (despite the negative indications of Sec. IV B) and at other points in the complex plane. Experience would indicate that without a good starting estimate of the location of a singularity we are unlikely to find solutions. At this time no conclusion seems possible as to whether or not the form (2.28) with additive singularities is a reasonable form for the LT χ.

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