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# NEW METHOD FOR CONFLUENT SINGULARITY ANALYSIS OF POWER SERIES

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## Abstract

A new method for calculating critical parameters from power series expansions, recently developed by the authors, is modified to take into account confluent singularities. The new procedure allows one to obtain wholly unbiased approaches to all physically meaningful critical parameters. The high-temperature, zero-field magnetic susceptibility series for the spin-1/2 Ising model for the face-centered cubic lattice is discussed as an illustrative example. Present results compare favorably with previously reported ones and agree closely with those from renormalization group theory.

## 1. Introduction

The high-temperature series (HTS) for the magnetic susceptibility of a spin crystal proves to be very useful in studying critical phenomena in magnetic models [1,2]. Phase transitions in such models take place as singularities in the thermodynamic functions. The determination of the set of parameters (critical parameters) characterizing such singularities is one of the main problems in the theory of critical phenomena (see the discussion, for instance, in ref. [3]).

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Close to the critical temperature $T_c$, the reduced zero-field susceptibility $\chi_0$ behaves approximately as (standard notation is used throughout this paper)

$$\chi_0 = a(T)(T - T_c)^{-\gamma}, \tag{1}$$

where $\gamma \geqslant 0$ is the critical exponent and $a(T)$ is a slow-varying function of the absolute temperature. Great effort has been devoted to obtaining the critical parameters $\gamma$ and $T_c$ and the form of $a(T)$ from the HTS [1,2]. Most studies have been performed on close-packed lattices. This is because these models are free from antiferromagnetic singular points, which make it difficult to handle the HTS [1,2]. In particular, the close-packed face-centred cubic (fcc) array is a favorite example because it is known to provide the best converged series for the thermodynamic functions [4]. Accordingly, we will restrict our discussion to the fcc spin-1/2 Ising model.

When the asymptotic form for $\chi_0$ is supposed to be strictly as in eq. (1), it is found that $\gamma_{HTS} \approx 1.250 \pm 0.002$, for the fcc spin-1/2 Ising model [1,5,6].

The critical exponent $\gamma = 5/4$ was believed to occur in all three-dimensional lattices. As a result, great controversy arose from the fact that an alternative theory, known as renormalization group theory (RGT) [7–10], predicted $\gamma_{RGT} \approx 1.240 \pm 0.001$ [7,8] or $\gamma_{RGT} \approx 1.241 \pm 0.004$ [9] for the same model. The RGT depends on the validity of speculative, yet reasonable, suppositions concerning the physics near the critical temperature. This theory predicts several scaling relationships among critical exponents, which are generally believed to be valid [10]. An extensive comparative study of this method and the procedure based on power series expansions has been carried out in order to test the RGT conclusions.

The disagreement between the results mentioned above is not due to numerical reasons, and it constitutes one of the most interesting problems in phase transition theory. The cause of the difference between the HTS and RGT values has been argued to be the disregard of some correction-to-scaling terms in eq. (1) [2,11,12]. The purpose of this work is to develop a method for computing critical parameters, taking into account the occurrence of these interfering terms.

A number of ways have been tried in order to trace such correction terms that are due to confluent singularities [13–19] (i.e. $a(T)$ is singular at $T = T_c$). Numerical investigation using Padé approximants [17], change of variables through different conformal mappings [18,19], and variants of the ratio method [13–16] suggest that the difference between $\gamma_{HTS}$ and $\gamma_{RGT}$ can be removed, and that the relationships predicted by the RGT are not violated. To obtain accurate enough results from the HTS, a fairly large number of expansion coefficients have been calculated for the fcc spin models [20,21], since they provide good test cases for the new techniques.

The aim of the present article is to propose an alternative method for obtaining critical parameters from HTS. To make clear its advantages, let us first discuss the drawbacks of the most widely used methods. For instance, Nickel [15] has pointed out that "below some critical number of series terms, Dlog Padé approximants do not have the resolution necessary to distinguish the presence of confluent correction terms, and will yield artificially stable but wrong estimates". The critical number of terms for the fcc spin-1/2 Ising model appears to be $N = 12$, and for this reason only the last three HTS terms, namely $N = 13, 14$, and 15 [20], are taken into account to estimate the critical parameters. Through appropriate extrapolation, Nickel [17] obtained $\gamma = 1.2346$ and, after rather subjective reasoning, concluded that $\gamma \approx 1.238 \pm 0.003$.

Procedures based on the ratio method [14–16] lead to more reliable conclusions. Zinn-Justin [14] obtained $\gamma \approx 1.245 \pm 0.003$ for the same spin model. As shown by McKenzie [16], the best converged ratio method sequences are obtained when the RGT exponents are used.

In summary, although the above-mentioned techniques enable one to distinguish the presence of corrections to scaling in spin-1/2 Ising models, they do not lead to accurate enough wholly independent estimates of the critical parameters.

We have recently developed a method for calculating critical parameters from power series expansions and applied it to some examples in statistical mechanics [22] and quantum theory [23]. This procedure is straightforward and enables simultaneous calculation of all the critical parameters. In addition to this, it is quite general and can be adapted to different problems. Close- and loose-packed-lattice spin–1/2 Ising models were discussed in ref. [22]. However, since the confluent singularities in the former case were not taken into account, the critical exponent for the fcc array was found to be $\gamma \approx 1.2467 \pm 0.0005$. It will be shown below that a modified version of our method leads to critical parameters in close agreement with the RGT ones, provided the correction-to-scaling terms are properly considered. The procedure is developed in sect. 2 and tested in sect. 3 on some simple mathematical functions showing confluent singularities as the closest ones to the origin. The method is applied to the HTS for the magnetic susceptibility of the fcc spin-1/2 Ising model in sect. 4. Conclusions are presented in sect. 5.

## 2. The method

Let $F(x)$ be a real function of the real variable $x$, so that it is representable as

$$F(x) = A(1 - x/x_0)^{-\gamma} + B(1 - x/x_0)^{-w} + \dots , \qquad \gamma \geqslant 0, \tag{2}$$

in a small neighborhood of $x_0$, the closest singularity to the origin. If $\gamma \geqslant w$, the second term in eq. (2) corresponds to the subdominant singular point. The real parameters $A$ and $B$ are called critical amplitudes and $\gamma$ and $w$ are the critical exponents. The Taylor series $F_0 + F_1 x + \dots + F_n x^n + \dots$ for $F(x)$ converges for all $|x| < |x_0|$.

Other singular terms that may appear in eq. (2) are supposed to contribute to a smaller degree than those above. In what follows, it is supposed that all higher-order terms of $F(x)$ in (2) have exponents differing from $-\gamma$ by a positive integer. It should be noticed that if $F(x) = g(x)(1 - x/x_0)^{-\gamma}$, then the function $g(x)$ must not be analytic in $x = x_0$ in order to have confluent singularities. If $g(x)$ is analytic in $x = x_0$, then the asymptotic behavior of $F(x)$ in the neighborhood of $x_0$ will be of the form (2), with $w = 0$ and $B = 0$.

The function

$$L(x) = (1 - x/u)^{\gamma'} \{F(x) - B'(1 - x/u)^{-w'}\} , \tag{3}$$

where $u$, $w'$, $\gamma'$, and $B'$ are real adjustable parameters, can be expanded in Taylor series about the origin with coefficients $L_n$ given by

$$L_n = \sum_{s=0}^{n} (-u)^{s-n} C(\gamma', n-s) \{F_s - B'(-u)^s C(-w', s)\} , \tag{4}$$

where $C(a, b) = a(a-1)(a-2)\dots(a-b+1)/b!$ are the combinatorial coefficients.

Because of the analytic properties of the function $F(x)$, if $u$, $\gamma'$, $w'$, and $B'$ were equal to $x_0$, $\gamma$, $w$, and $B$, respectively, then $L(x)$ would be analytic in a circle $C_R$ centered about the origin whose radius $R$ would be greater than $x_0$. In this case, $L(x)$ can be expanded as an infinite series of powers of $x$ (with coefficents given by (4)) which converges for $|x| < R > |x_0|$. A necessary condition to have such a convergent expansion is:

$$\lim_{n \to \infty} L_n x^n = 0, \quad |x| < R, \tag{5}$$

and in particular, as the series converges for $x = x_0$, we know from the D'Alembert ratio test:

$$x_0 \lim_{n \to \infty} |L_{n+1}/L_n| < 1. \tag{6}$$

Under the conditions already mentioned, eqs. (5) and (6) are exact and both satisfied simultaneously.

Up to now, of course, the critical parameters are unknown. However, they can be calculated approximately taking into account the requisites that the Taylor expansion of $L(x)$ must fulfill to be a convergent one, as discussed above. Let us consider the sequence

$$L(N, x) = \sum_{n=0}^{N} L_n x^n ; \tag{7}$$

when the adjustable parameters $u, \gamma', w'$, and $B'$ approach $x_0, \gamma, w$, and $B$, respectively, then conditions (5) and (6) imply

$$|L(N, x_0) - L(N+1, x_0)| < \epsilon, \quad \text{for all} \quad N > N^\star. \tag{8}$$

The smaller $\epsilon$ and $N^\star$ are, the better the convergence. This fact suggests that a set of optimum adjustable parameters could be obtained by determining them so that the best convergence condition is reached in eq. (8). It is reasonable to expect that such a condition would be found if the coefficients $|L_n|$ were as small as possible for growing $n$; in particular, the set of four equations $L_N = L_{N-1} = L_{N-2} = L_{N-3} = 0$ appears to provide a sensible criterion to determine the optimum approximation to the critical parameters. Since this can be done for each $N > 3$, we obtain sequences $u_N$, $\gamma'_N$, $w'_N$, and $B'_N$, which are expected to converge towards $x_0$, $\gamma$, $w$, and $B$, respectively, as $N$ tends to infinity. In addition, if $A'_N = L(N, u_N)$ were found to be convergent, its limit would have to be $A$.

The proposed set of equations can be considered as an extension of the necessary condition (5) for finite $n$, in order to provide the most rapidly convergent sequences.

Together with this calculation scheme, we will carry out another, computationally simpler one. If one of the equations of the above-mentioned set, say $L_{N-3} = 0$, is removed, then three of the four adjustable parameters can be expressed as functions of the remaining one. It is found that $B'_N$ depends strongly on $w'$ and exhibits a stationary point $((B'_N)_s)$. Therefore, it seems sensible to choose $w'_N$ to be such a stationary point. This criterion is particularly useful when $N$ is small, because in that case it is possible that roots for the system of four equations cannot be found. In addition, we will also try beforehand fixed $w'$ values to reveal the effect of the correction-to-scaling terms.

It can easily be verified that if $A$ and $B$ in eq. (2) are polynomials of degree $m$, then our procedure will yield the exact critical parameters for all $N \geqslant m$ when making the last four coefficients $L_N$ equal to zero [22,23]. We are unable to prove analytically whether the above criteria always lead to convergent sequences, but it will be tested numerically on a series of simple mathematical functions and a model of physical interest. To estimate the sequence limits, we use $1/N$ extrapolations or the Wynn-Shanks algorithm [24].

## 3. Application to some simple test functions

Let us consider some simple, but non-trivial, test functions having an asymptotic behavior, near the singularity closest to the origin, similar to eq. (2). The examples chosen are non-trivial in the sense that the coefficients $L_N$ are not identically zero for some $N > N^\star$, $N^\star > 1$.

The examples chosen here to apply our method are some hypergeometric functions (and functions related to them). The Taylor expansion for these functions,

$$ {}_2F_1(a, b; c; x) = \sum_{n=0}^{\infty} F_n x^n, \quad |x| < 1, \tag{9} $$

can easily be determined from the recurrence [25]

$$ F_{n+1} = F_n(a+n)(b+n)/(n+1)(c+n), \qquad n = 0, 1, 2, \ldots , $$

where $F_0 = 1$. Consequently, they represent an appropriate example to accomplish a careful analysis of convergence of the sequences corresponding to all critical parameters. The hypergeometric functions satisfy the following property [25]:

$$ \begin{aligned} {}_2F_1(a,b;c;x) = {} & \{\Gamma(c)\,\Gamma(c-a-b)/\Gamma(c-a)\,\Gamma(c-b)\}\; {}_2F_1(a,b;a+b-c+1;1-x) \\ & + (1-x)^{c-a-b}\,\{\Gamma(c)\,\Gamma(a+b-c)/\Gamma(a)\,\Gamma(b)\} \\ & \times\; {}_2F_1(c-a,c-b;c-a-b+1;1-x). \end{aligned} \tag{10} $$

From eq. (10), we can expect a dominant singularity at $x = 1$, with $\gamma = a + b - c$ for the critical exponent if the constants $a$, $b$, and $c$ take values so that all the arguments of the above gamma functions are not negative integers (cf. eq. (2)). In that case, eq. (10) shows that the critical behavior for these functions follows eq. (2), with critical amplitudes

$$ A = \Gamma(c)\,\Gamma(c-a-b)/\Gamma(c-a)\,\Gamma(c-b), $$

$$ B = \Gamma(c)\,\Gamma(a+b-c)/\Gamma(a)\,\Gamma(b), $$

and with $w = 0$ for the exponent of the interfering singularity. Observe that in this case, due to the fact that the hypergeometric functions are analytic at $x = 0$, the functions describing the amplitudes are analytic at $x = x_0 = 1$. Consequently, these first examples have only a critical remainder but not a true hierarchy of confluent singularities. However, they provide a first good test to show if, in a non-trivial case, our method confirms the prediction $w \to 0$ for the second critical exponent, in addition to the correct values for all other critical parameters.

As a first illustration, let us consider the case $a = b = 1$, $c = 3/4$, which presents the following asymptotic behavior:

$$ {}_2F_1(1, 1; 3/4; x) \approx A(1-x)^{-5/4} + B, \quad x \to 1^-, \tag{11} $$

with $A$ = 1.1107207 . . . and $B$ = 1/5. Table 1 shows all critical-parameter sequences, obtained upon using the method of sect. 2, including only the first forty Taylor coefficients. The results in table 1 were obtained following the first criterion of

Table 1

Critical-parameter sequences for the hypergeometric function ${}_2F_1(1, 1; 3/4; x)$. [Subdominant term is a critical remainder]

| $N$ | $\gamma'_N$ | $u_N$ | $A'_N$ | $B'_N$ | $-w'_N$ |
|---|---|---|---|---|---|
| 9 | 1.248763 | 0.9999739 | 1.11601 | −0.6420 | 0.3006 |
| 14 | 1.249638 | 0.9999953 | 1.11243 | 0.5629 | 0.1904 |
| 19 | 1.249835 | 0.9999984 | 1.11155 | 0.3160 | 0.1393 |
| 24 | 1.249908 | 0.99999932 | 1.111209 | 0.2596 | 0.1099 |
| 29 | 1.249942 | 0.99999965 | 1.111041 | 0.2361 | 0.0907 |
| 34 | 1.249961 | 0.99999980 | 1.110946 | 0.2236 | 0.0772 |
| 39 | 1.249971 | 0.99999987 | 1.110887 | 0.2161 | 0.0673 |

convergence (the last four coefficients $L_n$ vanish), but they are comparable to those derived by using the second criterion (extremum of $B'_N$ as a function of $w'_N$). The set of equations for the critical parameters was solved by the Newton–Raphson method. As is seen, after some lower-order oscillations, all critical parameters are obtained through monotonously converging sequences. A series of $1/N$ extrapolations from the results in table 1 give us the following estimations for the critical parameters: $x_0 = 1 \pm 10^{-7}$, $\gamma = 1.25000 \pm 5 \times 10^{-5}$, $A = 1.1107 \pm 10^{-4}$, $A' = 0.20 \pm 0.01$, and $-w = (1 \pm 10) \times 10^{-5}$, which show an acceptable agreement with the exact results (11). That is, both dominating terms at $x_0 = 1$ ($\gamma = 5/4$ and $w = 0$) are predicted simultaneously by means of a completely unbiased approach.

Let us consider a second and interesting example [25],

$$ {}_2F_1(1/4, 3/4; 1/2; x) = 2^{-1/2}(1-x)^{-1/2}\{1 + (1-x)^{1/2}\}^{1/2}, \tag{12a} $$

which presents the asymptotic behavior (cf. eq. (10)):

$$ {}_2F_1(1/4, 3/4; 1/2; x) \approx A(1-x)^{-1/2} + B, \tag{12b} $$

with $A = (1/2)^{1/2}$ and $B = (1/2)^{3/2}$. Function (12a) presents a true hierarchy of confluent singularities about $x_0 = 1$, but once again the subdominant term is a critical remainder ($w = 0$). We also tested the convergence of the sequences to the critical parameters characterizing this function, and results are displayed in table 2. The tabulated results were derived by applying the method of sect. 2 and by making use of

Table 2

Critical-parameter seuqneces for the hypergeometric function ${}_2F_1\,(1/4, 3/4; 1/2; x)$.
[Subdominant term is a critical remainder]

| $N$ | $\gamma'_N$ | $u_N$ | $A'_N$ | $B'_N$ | $-w'_N$ |
|---|---|---|---|---|---|
| 9 | 0.51400 | 1.000223 | 0.6442 | 0.3687 | 0.1034 |
| 14 | 0.50629 | 1.0000629 | 0.6766 | 0.3453 | 0.0668 |
| 19 | 0.50374 | 1.0000271 | 0.6881 | 0.3397 | 0.0493 |
| 24 | 0.50254 | 1.0000145 | 0.6938 | 0.3383 | 0.0390 |
| 29 | 0.50187 | 1.0000088 | 0.6970 | 0.3381 | 0.0323 |
| 34 | 0.50145 | 1.0000058 | 0.6991 | 0.3385 | 0.0276 |
| 39 | 0.50117 | 1.0000040 | 0.7006 | 0.3390 | 0.0240 |
| 44 | 0.50097 | 1.0000030 | 0.7016 | 0.3396 | 0.0213 |
| 49 | 0.50082 | 1.0000022 | 0.7024 | 0.3402 | 0.0191 |
| 54 | 0.50070 | 1.0000017 | 0.7030 | 0.3407 | 0.0174 |

the convergence criterion first mentioned. Notice that, as was the case with our first example (11), only the sequence converging to the subdominant critical amplitude $B$ shows an irregular convergence.

Standard $1/N$ extrapolation of the sequences in table 2 leads us to the following estimations for the critical parameters: $x_0 = 0.999998 \pm 3 \times 10^{-6}$, $\gamma = 0.49997 \pm 5 \times 10^{-4}$, $A = 0.708 \pm 10^{-3}$, $A' = 0.350 \pm 0.007$, and $w = (5 \pm 10) \times 10^{-3}$. As in the previous example, the agreement can be considered as fairly satisfactory, taking into account that all critical parameters have been obtained simultaneously.

We have also studied some other functions where an infinite number of confluent singularities is present, but having a critical exponent $w \neq 0$ for the leading subdominant term. For instance, the family of functions $\{F^{(t)}(x)\}$ given by

$$F^{(t)}(x) = 2^{-1/2}(1-x)^{-1/2}\{1+(1-x)^t\}^{1/2}, \tag{13}$$

satisfies the above requirements, and it contains as a particular case ($t = 1/2$) the hypergeometric function (12a). The asymptotic behavior of (13) near the critical singularity is similar to (12b); in fact, all the critical parameters of $F^{(t)}(x)$ coincide with those of (12a), except the exponent characterizing the leading confluent singularity, which in this case is $-w = t - 1/2$ instead of zero.

As a representative example, we display in table 3 the results obtained for the function with $t = 3/4$. In this case, we expect convergence to two leading confluent singularities with exponents $\gamma = 0.5$ and $-w = 0.25$. This function can be considered as a "hard" example to test our method because its Taylor coefficients do not reach their asymptotic behavior as quickly as in the previous examples with hypergeometric functions. This property is clearly revealed in table 3. The results displayed have also

Table 3

Critical-parameter sequences for the function (13) ($t$ = 3/4).
[An infinite number of confluent singularities is present; subdominant term has a critical exponent $-w$ = 1/4]

| $N$ | $\gamma'_N$ | $u_N$ | $A'_N$ | $B'_N$ | $-w'_N$ |
|---|---|---|---|---|---|
| 9 | 0.50253 | 1.000224 | 0.70223 | 0.649 | 0.3229 |
| 19 | 0.49817 | 0.9999733 | 0.71425 | 0.980 | 0.3893 |
| 29 | 0.49898 | 0.9999906 | 0.71142 | 0.7220 | 0.3534 |
| 39 | 0.49936 | 0.9999958 | 0.70996 | 0.6156 | 0.3309 |
| 49 | 0.49955 | 0.9999977 | 0.70917 | 0.5605 | 0.3168 |
| 59 | 0.49967 | 0.9999986 | 0.70869 | 0.5269 | 0.3072 |

been obtained following the first convergence criterion discussed in sect. 2. Once again, after an oscillation the convergence becomes smooth ($N > 19$); this fact simplifies the extrapolation of sequences. By making use of linear and parabolic $1/N$ extrapolations, we obtain the following estimations for the critical parameters: $x_0$ = $1.000002 \pm 3 \times 10^{-6}$, $\gamma = 0.5003 \pm 4 \times 10^{-4}$, $A = 0.707 \pm 10^{-3}$, $A' = 0.36 \pm 0.02$, and $-w = 0.254 \pm 0.006$. Although the exponent $w$ is not predicted with the same accuracy as was done for the previous examples (11) and (12), the whole set of critical parameters can be considered as acceptably described.

The results obtained for other functions (13) with different values of $t$ are similar in accuracy. The same holds when employing the criterion based on following the extremum of $B'_N$ as a function of $w'_N$ ($(B'_N)_s$). In this latter case, we find that the best approximation is obtained when $N = N^\star$, so that $(B'_{N^\star})_s$ is an extremum over $N$. This criterion provides results of comparable accuracy to those displayed in tables 1–3, but involving a lower number of Taylor coefficients. This alternative might be valuable when a large number of coefficients is not available for the function of interest.

The analysis performed above with these very simple, but non-trivial functions suggests that the method proposed in sect. 2 would be useful in predicting the whole set of critical parameters of problems having confluent singularities. Even though convergence has not been proved analytically, it has been tested numerically for some different and representative functions. Results appear to be accurate enough to provide acceptable, completely unbiased estimations of both dominant and subdominant critical exponents. In the next section, we apply this method to a more relevant, and controversial, physical model.

## 4. Analysis of the high-temperature susceptibility series for the spin-1/2 fcc-lattice Ising model

Near the phase transition, the reduced magnetic susceptibility for the spin Ising models is supposed to behave approximately as $F(x)$ in eq. (2), where $x = \tanh(J/kT)$ and $x_0 = x(T_c)$ (standard notation is used [1]). In addition, $\chi_0$ can easily be expanded in powers of $x$ [1] and in the case of the fcc lattice, there are sixteen available coefficients. We can therefore apply the method previously outlined and obtain the critical parameters.

In order to make clear the influence of the corrections-to-scaling, we have tried several calculation schemes with fixed $w'$ values:

(a) $w' = 0$. This choice does not take into account the confluent singular point, and the results so obtained can be compared with those in refs. [1,4,5, and 22].

(b) The confluent singularity is disregarded, but the Taylor expansion about $x_0$ of a temperature-dependent critical amplitude is supposed to originate in the second term of eq. (2) (see sect. 2). In this case, we could set $w = \gamma - 1$. Since changes in $w'$ of about 5% do not appreciably alter the results, we set $w' = 1/4$ (corresponding to $\gamma = 5/4$).

(c) A subdominant singular point with exponent $\Delta_1$ is considered and therefor $w = \gamma - \Delta_1$. Since $\Delta_1 = 0.50 \pm 0.02$ [7,8] (probably $\Delta_1 = 0.496$ [16]) according to the RGT, we choose $w' = 3/4$, which corresponds to $\gamma = 5/4$ and $\Delta_1 = 1/2$.

The $\gamma'$ and $u$ sequences are shown in table 4, from which we can draw the following conclusions:

(a) When $w' = 0$, the critical exponent sequence appears to tend towards 5/4 when $N \leqslant 9$ and then decreases as $N$ increases. This is due to the fact that the subdominant singularity has no distinguishable effect on the low-order Taylor coefficients, as argued by Nickel [17]. This sequence seems to approach $\gamma = 1.245$, in agreement with Zinn-Justin's results [14,15]. However, a $1/N$ extrapolation yields $\gamma = 1.2431$.

(b) The critical exponent sequence when $w' = 1/4$ is similar to the previous one and its limit, estimated through $1/N$ linear extrapolation, is approximately found to be 1.2429. Clearly, the temperature dependence of the critical amplitude has no remarkable effect on the results.

(c) When $w' = 3/4$, a critical exponent close to the RGT result is obtained, suggesting that the corrections-to-scaling are the cause of the difference between HTS and RGT estimates.

We deem that these results are more conclusive than McKenzie's [16] regarding the difference between $\gamma_{HTS}$ and $\gamma_{RGT}$. However, it is still necessary to show that our procedure itself leads to the actual subdominant critical parameters. To this end, let $w'$ take its optimum value freely as discussed in sect. 2. The results in table 5,

Table 4

$\gamma'$ and $u$ sequences (first and second figure, respectively) for fixed $w'$ values, corresponding to the spin-1/2 fcc-lattice Ising model

| $N$ | $w' = 0$ | $w' = 0.25$ | $w' = 0.75$ |
|---|---|---|---|
| 8 | 1.248659<br>0.10174329 | 1.249185<br>0.10174528 | 1.251874<br>0.10175149 |
| 9 | 1.250644<br>0.10175606 | 1.251560<br>0.10175903 | 1.256204<br>0.10176817 |
| 10 | 1.248282<br>0.10174274 | 1.248436<br>0.10174317 | 1.249203<br>0.10174472 |
| 11 | 1.246312<br>0.10173283 | 1.245952<br>0.10173193 | 1.244176<br>0.10172928 |
| 12 | 1.245341<br>0.10172843 | 1.244791<br>0.10172719 | 1.242070<br>0.10172354 |
| 13 | 1.244996<br>0.10172701 | 1.244429<br>0.10172584 | 1.241614<br>0.10172241 |
| 14 | 1.244872<br>0.10172654 | 1.244338<br>0.10172553 | 1.241679<br>0.10172255 |
| 15 | 1.244737<br>0.10172607 | 1.244224<br>0.10172518 | 1.241669<br>0.10172253 |

Table 5

Critical-parameter sequences for the dominant and subdominant singular points in the spin-1/2 fcc-lattice Ising model ($\Delta_{1,N} = \gamma'_N - w'_N$)

| $N$ | $\gamma'_N$ | $u_N$ | $-(B'_N)_s$ | $A'_N$ | $\Delta_{1,N}$ |
|---|---|---|---|---|---|
| 11 | 1.24450 | 0.10172961 | 0.02312 | 0.983743 | 0.5443 |
| 12 | 1.24249 | 0.10172393 | 0.03774 | 0.991195 | 0.5346 |
| 13 | 1.24198 | 0.10172271 | 0.04120 | 0.993262 | 0.5269 |
| 14 | 1.24196 | 0.10172277 | 0.04081 | 0.993544 | 0.5200 |
| 15 | 1.24188 | 0.10172268 | 0.04098 | 0.993892 | 0.5136 |

obtained following the stationary point criterion, show plainly that the present method leads to critical exponents of both dominant and subdominant singular points, with values close to those predicted by the RGT. As far as we know, there is no unbiased HTS calculation of the corretion-to-scaling terms reported previously. When applying the first criterion discussed in sect. 2, we have found no zeroes for the system of four equations in the region of interest, except for $N$ = 14 and 15. In this latter case, the results are: $u = 0.10172236$, $\gamma' = 1.24140$, $\gamma' - w' = 0.4667$, $A' = 0.99684$, and $B' = -0.04157$, which are in acceptable agreement with results in table 5.

Since we do not know the appropriate extrapolation algorithm for our sequences, we try visual and analytical $1/N$ extrapolations (linear and parabolic) as well as the Wynn-Shanks algorithm [24]. On averaging the most unfavorable limit estimate for each sequence in table 5, with the last term in it (approximation to $N^{\star}$, see sect. 3), we obtain

$$x_0 = 0.101721 \pm 10^{-6}, \qquad \gamma = 1.241 \pm 0.002,$$

$$\Delta_1 = 0.49 \pm 0.03, \qquad A = 0.996 \pm 0.003,$$

$$-B = 0.042 \pm 0.002.$$

Since the error bounds are very conservative, present critical parameters could probably be the most accurate ones, calculated by means of an unbiased analysis of the HTS. The critical amplitudes $A$ and $B$ were previously only roughly estimated, through biased approaches that profit from the RGT critical exponents [16]. The above $x_0$ value is one figure more accurate than the most accurate ones in the literature [5,6]. Furthermore, the agreement found between the HTS and RGT analyses seems to confirm the results reported for other three-dimensional lattices, obtained following different procedures [26]. It is expected that present results can be considerably improved by adding more terms to the HTS.

## 5. Conclusions

A method has been developed for calculating critical parameters from power series expansions. It has been shown that if correction-to-scaling terms are properly taken into consideration, the estimated $\gamma_{HTS}$ agrees with $\gamma_{RGT}$. The originality of the present procedure is that the critical parameters of both the dominant and sub-dominant singularities are simultaneously calculated.

Our technique is suitable for dealing with many problems of actual physical interest [22,23]. It is only necessary to have a large enough number of Taylor coefficients and to know the proper asymptotic form for the function near the singular point.

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*Note added in proof*

After submitting this work, an interesting article by P.R. Graves-Morris on confluent singularities has been published (J. Phys. A21(1988)1867). His numerical results for the critical parameters are in agreement with those obtained in this article.

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