Method of analysis of critical-point singularities from power-series expansions

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(Received 19 June 1985)

A simple method is proposed for determining characteristic parameters of critical-point singularities from power-series expansions. It applies to a broad class of functions of physical interest and provides acceptable, simultaneous approximations to the critical point, exponent, and amplitude. Several examples of low- and high-temperature series expansions for thermodynamic properties of spin- $\frac{1}{2}$ Ising models are studied, and quite accurate results are obtained for both close- and loosepacked arrays.

I. INTRODUCTION

Exact solutions to problems in theoretical physics are rarely attainable. Approximations are often given as power-series expansions that in most cases are divergent or at least have finite convergence radii. Owing to this, great effort has been devoted to the development of appropriate techniques for handling such series.

Power-series expansions with finite convergence radii nowadays are of great interest in theoretical physics and chemistry. Among them we can mention low- and hightemperature expansions for some thermodynamic properties (such as magnetization, magnetic susceptibility, and specific heat) of the spin- $\frac{1}{2}$ Ising and Heisenberg models,¹⁻³ virial expansions for simple real gas models,⁴ series in inverse powers of the nuclear charge for the electronic energy of atoms,⁵ and power-series expansions for the energy eigenvalues of rigid polar rotators in electric fields (see, for example, Ref. 6 and references therein).

Sometimes the physical value of the expansion parameter lies outside the convergence region, which makes necessary the use of convenient summation methods. In other cases (i.e., in the study of critical behavior in lattice statistics) the singularity determining the convergence radius has itself some physical meaning. Due to this, great effort has been devoted to the determination of the characteristics of the singularities of a function from its power-series expansion.

The purpose of the present paper is to develop a very simple procedure for simultaneous calculation of all critical parameters. As far as we know, none of the currently used techniques exhibit such an advantageous feature that in some cases is of paramount importance, as shown below. The method is presented in Sec. II. Phase transitions for the magnetization and magnetic susceptibility of a number of two- and three-dimensional close-packed spin- $\frac{1}{2}$ models are studied in Sec. III. The procedure is modified in Sec. IV to deal with loose-packed systems. Finally, other problems that can be treated this way are briefly discussed in Sec. V.

II. THE METHOD

As stated before, the aim of this paper is to develop a systematic procedure for determining characteristic pa-

rameters of critical-point singularities from power-series expansions. To this end let us consider a function F(x)with singularities at x_0, x_1, x_2, \ldots , where $|x_0| < |x_1| \le |x_2| \le \cdots$. The Taylor-series expansion $F_0 + F_1 x + F_2 x^2 + \cdots$ for F(x) converges in $|x| < |x_0|$ and

$$\lim_{n \to \infty} |F_n / F_{n+1}| = |x_0| .$$
 (1)

The present method applies when a critical (real) exponent a exists so that the "factorized" function

$$f(x) = (1 - x/x_0)^a F(x)$$
(2)

is analytic in $|x| < |x_1|$, and $A = f(x_0)$, the critical amplitude or singularity amplitude, is non-null. For the sake of simplicity it is assumed that x_0 is real though complex x_0 values can be treated the same way.

In order to obtain x_0 , a, and A simultaneously, we define

$$g(u,b,x) = (1 - x/u)^{b} F(x)$$
, (3)

where u and b are adjustable parameters. On expanding the right-hand side of Eq. (3) in powers of x we obtain

$$g(u,b,x) = \sum_{n=0}^{\infty} g_n(u,b) x^n , \qquad (4a)$$

where

$$g_{n}(u,b) = \sum_{s=0}^{n} \binom{b}{s} (-u)^{-s} F_{n-s} , \qquad (4b)$$

and $\binom{b}{s}$ are the binomial coefficients.

Clearly, if $u = x_0$ and b = a the sequence

$$g(N,u,b,x) = \sum_{n=0}^{N} g_n(u,b) x^n, \quad N = 1,2,3,\ldots$$
(5)

will converge towards f(x) in $|x| < |x_1|$. In particular, $g(\infty, x_0, a, x_0) = A$. From a practical viewpoint, proper u and b values are set so that the largest convergence rate for the sequence (5) is obtained. A sensible convergence criterion seems to be

$$g_N(u_N, b_N) = g_{N-1}(u_N, b_N) = 0$$
, $N = 1, 2, 3, ...$ (6)

from which we obtain the u and b values for each N

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value. If the sequences u_N , b_N , and $A_N = g(N, u_N, b_N, u_N)$ (N = 1, 2, 3, ...) are found to be convergent, their limits must be x_0 , a, and A, respectively.

Although we do not give either a rigorous proof of convergence or a mathematical justification of the choice (6), the method is very reliable because the convergence of three sequences is tested simultaneously. Therefore, fortuitous convergence is very improbable. Our assumptions will be numerically checked in Secs. III and IV. Besides, it is very easily shown that Eq. (6) leads to the exact result when f(x) is a polynomial function of degree N-2 in which case $g_M(u_N, b_N) = 0$ for all M > N-2.

The roots of Eq. (6) are easily calculated by means of the Newton-Raphson method^{7,8} and the sequences u_N , b_N , and A_N are simultaneously obtained. This fact is of great importance because it is known that the use of previously computed x_0 and a values in calculating A leads to inaccurate results if the input is not very accurate.⁹

Several ways of estimating x_0 and a have been proposed. Among them we can mention the following: (a) the ratio method and its several related variants^{1,2,9-11} that obtain the limit (1) by means of an appropriate asymptotic expression for F_n ; (b) some techniques using Padé approximants, the most successful of which requires a previous accurate calculation of one of the critical parameters;¹² (c) methods of sequence extrapolation such as the Neville table^{9,13} and the Wynn-Shanks ϵ algorithm,^{14,15} the latter giving reasonable approximations to a and x_0 from the power series for $\ln F$ and $d \ln F/dx$, respectively; (d) procedures based upon the Borel transform and its variants;^{16,17} and (e) the contour-map method.^{9,18,19} Some of these procedures require the use of different functions derived from F(x) in order to calculate x_0 and a. In the present case both critical parameters are obtained from the Taylor expansion for F(x).

The contour-map method^{9,18,19} is particularly interesting because it resembles the present one. It applies when $x_0 = -x_1 > 0$ and consists of defining the function

$$h(m,u,b,x) = \left(1 - \frac{x}{u}\right)^{b} \left(1 + \frac{x}{u}\right)^{m} F(x) .$$
 (7)

Different u and b values are tried for m = 0, 1, 2, ... so that the Taylor coefficients for h decrease in magnitude and alternate in sign. The uncertainty in the computed x_0 and a values decreases as m increases. When there is only one singularity closest to the origin, the function F(x) in (7) is replaced by F(x)F(-x). However, in this last case results are considerably poorer. On the other hand, our method applies successfully to both cases as shown in Secs. III and IV provided it is properly modified when $x_1 = -x_0 < 0$.

Numerical investigation shows that the present method applies even when f(x) has a branch-point singularity at x_0 . Although at present there is not a plausible mathematical justification, it seems that the sequences u_N , b_N , and A_N converge even when the Taylor series for f(x) at $x = x_0$ does not. For example, convergence of the sequences is observed when $F(x) = (1 - x/x_0)^{-a}$ $+(1 - x/x_1)^{-t}$ where a and t are positive nonintegers (a > t) and $0 < x_0 \le x_1$. Obviously, in this case $f(x)=(1-x/x_0)^a F(x)$ is not analytic at x_0 . For the particular case $a=\frac{3}{2}$, t=1, and $x_0=x_1=1$ we obtain (N=70) $a=1.49\pm0.01$, $x_0=1.00002\pm0.00002$, and $A=1.1\pm0.1$, which agree with the exact values.

III. APPLICATION TO CLOSE-PACKED-LATTICE SPIN- $\frac{1}{2}$ MODELS

The spontaneous magnetization for a two-dimensional square spin- $\frac{1}{2}$ Ising model is known to be^{9,20-23}

$$M(x) = (1+x)^{1/4}(1-x)^{-1/2}(1-6x+x^2)^{1/8}, \qquad (8)$$

where $x = \exp(-4J/kT)$, k being the Boltzmann constant, T the absolute temperature, and J the spin-spin interaction (coupling constant). This model is a good test problem since its critical parameters are exactly known. In fact, it has recently been used to check the ϵ algorithm.^{14,15}

The singularities of M(x) are at $x_0=3-2^{3/2}$, $x_1=1$, $x_2=-1$, and $x_3=3+2^{3/2}$, and its low-temperature series expansion converges in $|x| < x_0$. [The coefficients of the x-power-series expansion for M(x) are easily calculated.] The closest singularity to the origin, x_0 , is related to the critical temperature T_c (Curie temperature) of the phase transition.

On applying the present method it is found that the errors $|a-b_N|$, $|x_0-u_N|$, and $|A-A_N|$ are smaller than 10^{-14} for $N \ge 23$. Notice that the three critical parameters have been obtained with the same accuracy, which does not happen when using other techniques.

The reduced magnetic susceptibility χ can be approximated by low- and high-temperature expansions.^{9,20} Only the latter will be considered here because it has been the most frequently studied (see Ref. 20 and references therein). This series is of the form

$$\chi = \sum_{n=0}^{\infty} \chi_n x^n , \qquad (9)$$

where $x = \tanh(J/kT)$. The coefficients χ_n for some lattice arrays can be found in Ref. 20.

The singularity of $\chi(x)$ closest to the origin for closepacked lattices (ferromagnetic singularity $x_0 > 0$) factors as indicated in Eq. (2).¹⁻³ On the other hand, the magnetic susceptibility for loose-packed arrays is singular at $x_0 > 0$ and $x_1 = -x_0$ (antiferromagnetic singularity), due to which they are studied in Sec. IV.

The close-packed arrays to be studied here are the twodimensional plane-triangular (PT) and the threedimensional face-centered-cubic (fcc) lattices. Let us first consider the former. The first 16 coefficients χ_n for the PT Ising model obtained by Domb²⁰ have been used to build the sequences b_N , u_N , and A_N in Table I. They seem to converge and, as usually happens,¹³ u_N approaches the limit more quickly than the others. The contour-map method¹⁹ enables one to calculate only x_0 and *a* and its results are less accurate than those estimated from Table I.

In order to obtain closer approximations to the limits of the sequences we have tried two convergence-accelerating

N	b_N	u _N	A_N
13	1.749 27	0.267 943 9	0.848 80
14	1.749 09	0.267 941 9	0.849 12
15	1.749 28	0.267 943 9	0.848 76
16	1.749 47	0.267 945 8	0.848 39

TABLE I. Sequences for the magnetic susceptibility for the two-dimensional plane-triangular Ising model.

techniques, namely, the ϵ algorithm (EA) (Refs. 14, 15, and 24–26) and an N^{-1} extrapolation (E), using the last terms of the sequences. Since these procedures are widely used they require no further comment. Similar results are obtained in both cases as shown below.

For the critical exponent we have $a \simeq 1.7492$ (EA) and $a \simeq 1.7503$ (E) which agree with the exact exponent value $a = \frac{7}{4}$, which is supposed to occur in all two-dimensional lattices. The present estimate for x_0 is $x_0 \simeq 0.267942$ (EA) and $x_0 \simeq 0.267954$ (E), the exact result being $x_0 = (2+3^{1/2})^{-1} = 0.2679492...$ The A values obtained in this paper, $A \simeq 0.8491$ (EA) and $A \simeq 0.8467$ (E), agree with that coming from the ratio method (using exact x_0 and a values)⁹ and other procedures:^{27,28} $A = 8472 \pm 0.0002$. It is worth noting that much more accurate critical parameters are obtained if at least one of them is exactly known. However, we do not profit from this fact because the present method is developed to deal with more realistic models where no exact critical parameters are even to exact critical parameters are even to exact critical parameters are not exact critical parameters are even to exact critical parameters are even to exact critical parameters are even to exact critical parameters are even the even to the even the eve

Table II shows the sequences for the critical parameters of the fcc Ising model constructed from the first 12 coefficients χ_n ²⁰ The critical parameters obtained directly from Table II are more accurate than those coming from the contour-map method.¹⁹ Besides, our results can be improved by using the aforesaid convergence-accelerating techniques. Α straightforward calculation yields $a \simeq 1.2462$ (E), $a \simeq 1.2473$ (EA), $x_0 \simeq 0.101729$ $x_0 \simeq 0.101731$ (EA), $A \simeq 0.9753$ (E), and $A \simeq 0.9675$ (EA) which agree with the results obtained through other methods: $a = \frac{5}{4}$ (which is supposed to occur in all three-dimensional arrays), $x_0.10175 \pm 10^{-5}$, 9,20 and A = 0.963 $\pm 0.002.^{20}$

Although more accurate results than the present ones are available, we deem that our method is interesting because it is very simple and enables simultaneous calculation of all the critical parameters. Besides, it poses a novel way of approaching the problem of critical behavior and offers some advantages as shown in Sec. IV.

In order to show that the convergence of the sequences

TABLE II. Sequences for the magnetic susceptibility for the three-dimensional face-centered-cubic Ising model.

N	b_N	<i>u</i> _N	A_N	
9	1.247 66	0.101 739 2	0.972 48	
10	1.247 76	0.101 740 1	0.972 30	
11	1.247 56	0.101 738 5	0.972 69	
12	1.247 28	0.101 736 4	0.973 23	

TABLE III. Sequences for the magnetic susceptibility for the three-dimensional face-centered-cubic Heisenberg model.

N	b_N	<i>u</i> _N	A_N
6	1.304 24	0.245 13	1.269 51
7	1.398 39	0.248 10	1.113 68
8	1.527 60	0.25107	0.897 25
9	1.506 95	0.250 67	0.931 83

is not fortuitous or model dependent we now consider the magnetic susceptibility for the fcc spin- $\frac{1}{2}$ Heisenberg model.²⁹ The sequences for the critical parameters displayed in Table III were obtained from the first nine coefficients χ_n of the series in powers of x=J/kT.²⁹ They appear to converge more slowly than those studied previously and therefore the results are expected to be less accurate. In this case we have (only N^{-1} extrapolation has been tried) $a\simeq 1.4$, $x_0\simeq 0.25$, and $A\simeq 1.10$ that agree with $a=1.43\pm0.01$ and $x_0=0.249\pm10^{-3}$ (Ref. 29) and with $a\simeq 1.406$ and $x_0\simeq 0.245$.¹⁵ As far as we know the A value was not reported previously.

IV. APPLICATION TO LOOSE-PACKED-LATTICE ISING MODELS

It is well known that the magnetic susceptibility for the loose-packed-lattice Ising models has two closest singularities to the origin that correspond to the ferromagnetic $(x_0 > 0)$ and antiferromagnetic $(x_1 = -x_0)$ phase transitions.³ Owing to the presence of the antiferromagnetic singularity the sequences u_N , b_N , and A_N as defined in Sec. II exhibit a characteristic odd or even superimposed oscillation that leads to too rough estimations of the critical parameters. However, the procedure of Sec. II is still useful since it reveals the existence of the singularity at $-x_0$.

In this section we study the high-temperature magnetic-susceptibility series $[x = \tanh(J/kT)]$ for the body-centered-cubic (bcc) and simple-cubic (sc) Ising models. The Taylor coefficients χ_n are given in Ref. 20.

The sequences u_N , b_N , and A_N for the bcc lattice are shown in Table IV as an illustrative example. On estimating the limits of the odd and even sequences separately and then averaging the results we obtain $a \simeq 1.3 \pm 0.3$ and $x_0 \simeq 0.154 \pm 0.004$ that agree poorly with the much more accurate results $a \simeq 1.25$ and $x_0 \simeq 0.1562$.⁹

It is clear that the antiferromagnetic singularity has to be taken into account explicitly, as in the case of the contour-map method,¹⁹ in order to obtain acceptable re-

TABLE IV. Sequences for the magnetic susceptibility for the body-centered-cubic Ising model (method of Sec. II).

N	b_N	u _N
12	1.735 84	0.136 82
13	1.026 02	0.153 48
14	1.721 36	0.13907
15	1.028 12	0.153 86

sults. To this end let us suppose that the magnetic susceptibility for the above-mentioned three-dimensional Ising models can be written as 20,28

$$\chi(x) = f_1(x)(1 - x/x_0)^{-a} + f_2(x)(1 + x/x_0)^{a'}, \quad (10)$$

where |a| > |a'| and $f_1(x)$ and $f_2(x)$ are analytic in $-x_0 < x \le x_0$ and $-x_0 \le x \le x_0$, respectively. The ferromagnetic and antiferromagnetic amplitudes are defined as $A = f_1(x_0)$ and $A' = f_2(x_0)$, respectively.

The odd and/or even superimposed oscillation of the sequences must approximately be due to a contribution of the form $A'(1+x/x_0)^{a'}$. To remove it we define

$$F(x) = \chi(x) - v(1 + x/u)^{a'}, \qquad (11)$$

and

$$g(u,b,v,x) \equiv (1-x/u)^{b} F(x)$$
 (12)

From the Taylor series for g(u,b,v,x) we build the sequence of partial sums

TABLE V. Sequences for the magnetic susceptibility for the body-centered-cubic Ising model (method of Sec. IV).

N	b _N	u _N	U _N	A_N
12	1.21649	0.155 918	0.51095	1.062 66
13	1.21397	0.155 889	0.51317	1.067 97
14	1.221 50	0.155 973	0.527 49	1.052 27
15	1.219 59	0.155 955	0.529 11	1.056 59

$$g(N,u,b,v,x) = \sum_{n=0}^{N} g_n(u,b,v) x^n , \qquad (13)$$

and the values of the parameters u, b, and v are set so that

$$g_{N-2}(u_N, b_N, v_N) = g_{N-1}(u_N, b_N, v_N)$$

= $g_N(u_N, b_N, v_N) = 0$, (14)

for $N = 2, 3, 4, \ldots$.

It immediately follows from $g_{N-2}(u_N, b_N, v_N) = 0$ that

$$v_N = \left[\sum_{n=0}^{N-2} (-1)^n \binom{b_N}{n} u_N^{N-n-2} \chi_{N-n-2}\right] / \left[\sum_{n=0}^{N-2} (-1)^n \binom{b_N}{n} \binom{a'}{N-n-2}\right],$$
(15)

and the Newton-Raphson method is used to obtain u_N and b_N from the remaining algebraic equations. Obviously, the critical parameters x_0 , a, A, and A' are the limits of the sequences u_N , b_N , $A_N = g(N - 3, u_N, b_N, v_N, u_N)$, and v_N , respectively, provided they converge.

The exact antiferromagnetic critical exponent is known to be $a' = \frac{7}{8}$ (Refs. 20 and 28) and for the sake of simplicity we use this value in the present paper. If it were unknown we could calculate it simultaneously with the other critical defining parameters by $F(x) = \chi(x) - v(1 - x/u)^c$ and then solving g_{N-3} $=g_{N-2}=g_{N-1}=g_N=0$ (N=3,4,5,...) for u_N , b_N , v_N , and c_N . The last sequence will converge towards a'.

The sequences for the bcc lattice are given in Table V. Upon comparing Tables IV and V we notice that the use

of (11) greatly reduces the odd or even oscillation leading to quickly converging sequences.

As stated before, simultaneous calculation of all the critical parameters is of great importance because too much manipulation of the power series may lead to inaccurate results. This is the case of the antiferromagnetic amplitude that could only be roughly estimated,^{20,28} and the results obtained do not appear to very reliable. The present method yields A' values that are as accurate as the A values. We deem that our A' values are the most accurate reported in the literature up to now.

Standard graphical and numerical polynomial extrapolations have been used to estimate the limits of the sequences u_N , b_N , v_N , and A_N . Present critical parameters compare favorably with the most accurate ones reported

TABLE VI. Magnetic-susceptibility critical parameters for loose-packed-lattice Ising models.

Model	Method	а	x 0	A	Α'
bcc	Present	1.250±0.004	0.156 12±0.000 04	0.966±0.006	0.609±0.005
	Padé (Ref. 19)	1.250 ± 0.004	0.1562 ± 0.0002		
N = 15	Ref. 19	1.250 ± 0.01	0.1562 ± 0.0002		
	Refs. 20 and 27 ^a		0.15612 ± 0.00003	0.965 ± 0.003	0.536, 0.622
sc	Present	1.250 ± 0.002	0.218 15±0.000 04	1.016±0.004	0.644±0.004
	Padé (Ref. 19)	1.250 ± 0.004	0.2182 ± 0.0003		
N = 17	Ref. 19	1.249 ± 0.02	0.21812 ± 0.00004		
	Refs. 20 and 27 ^a		0.21813 ± 0.00001	1.016±0.001	0.561, 0.630

*The exact a value is used.

in the literature as shown in Table VI. There is great disagreement in the case of A' but we consider that our A' values are highly reliable because the sequence v_N is as smooth as A_N (see Table V) and our A values are in close agreement with those reported in Ref. 19. This is one of the advantages of the simultaneous calculation of the critical parameters. In addition to this, the present method is simpler and more straightforward than any other that yields results of the same accuracy.

The magnetic susceptibility for the two-dimensional loose-packed lattices has a logarithmic antiferromagnetic singularity.²⁰ It is believed that $\chi(x)$ is of the form

$$\chi(x) = f_1(x)(1 - x/x_0)^{-a} + f_2(x)(1 + x/x_0)\ln(1 + x/x_0), \qquad (16)$$

due to which F(x) has to be defined as $\chi(x) - v \ln(1 + x/u)$ in order to apply the present method. The calculation is similar to that discussed above.

V. FURTHER COMMENTS AND CONCLUSIONS

A method for studying critical behavior was developed that applies successfully to a wide class of physically interesting nonanalytic functions. Its main advantage is to allow simultaneous calculation of all the critical parameters, which leads to very reliable results. The procedure developed in Secs. II and IV applies to other problems in theoretical physics and chemistry than those discussed here. As an example, let us consider the Mathieu equation³⁰

$$\Psi''(\theta) + [E(\lambda) - \lambda \cos\theta] \Psi(\theta) = 0 , \qquad (17)$$

where $\Psi(\theta + \pi) = \Psi(\theta)$. On taking into account wellknown results³⁰⁻³² one can argue that the characteristic values $E(\lambda)$ are of the form $E(\lambda)=F_1(\lambda)$ $+(1+\lambda^2/\lambda_0^2)^{1/2}F_2(\lambda)$, where $\lambda_0^2 > 0$ and $F_1(\lambda)$ and $F_2(\lambda)$ are analytic in $|\lambda| < R > |\lambda_0|$. The coefficients of the λ -power-series expansion for $E(\lambda)$ is available³⁰ and the present method applies to $E(\lambda)-E(\lambda_0)$. The critical parameters λ_0 , $F_1(\lambda_0)$, and $F_2(\lambda_0)$ can be simultaneously calculated in a way similar to that shown in Sec. IV. Results for this and other problems will be presented in a forthcoming paper.

ACKNOWLEDGMENTS

INIFTA is a research institute jointly established by the Universidad Nacional de La Plata, the Consejo Nacional de Investigaciones Científicas y Técnicas, and the Comisión de Investigaciones Científicas de la Provincia de Buenos Aires, Argentina.

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