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CRITICAL PARAMETERS FROM POWER SERIES EXPANSIONS

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Abstract

A simple and quite general method is developed for calculating critical parameters from power series expansions. The series coefficients of the problem function are introduced into a properly parametrized recurrence relationship. As a result, sequences are obtained that converge towards the critical parameters characterizing the closest singularity to the origin. The low-temperature series for the thermodynamic functions of spin-1/2 Ising models are discussed. Results are shown for the interfering, nonphysical singularities of the face-centred cubic and body-centred cubic lattices. The determination of these singularities would allow their factorization previous to the study of the physically important ones.

1. Introduction

The study of critical phenomena has attracted a great deal of attention during the last century. However, the development of a unified and sound theory to analyze such phenomena is, comparatively, a recent achievement (see ref. [1] for a review of the historical development and present status of the theory).

Phase transitions appear in different types of systems. For instance, in solid-state physics, magnetic transitions are of particular interest, whereas fluid-solid phase transitions are relevant to different areas of physics and chemistry. In this paper, we are concerned mostly with the first class of phenomena. However, both can be related owing to the existence of symmetries between changes of magnetic state and changes of aggregation state [2].

In order to analyze theoretically any of the above phenomena, one must first propose a model for them. Spin-lattice models (including the so-called Ising, Heisen-

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berg, and $X-Y$ models, among others) are a favorite tool to study magnetic transitions [3,4]. On the other hand, imperfect-gas continuum [5–8] and lattice [9,10] models have been used to mimic the behavior of systems exhibiting condensation or solidification. In particular, the models with hard-core repulsive interactions [5–8], as well as Lennard–Jones interactions ([11] and references quoted therein), seem to be useful in trying to interpret the real behavior.

Critical phenomena are characterized by the occurrence of singularities in some thermodynamic functions or their derivatives. Let us consider one example, relevant to our discussion later on, to illustrate this point. Suppose that H is the Hamiltonian describing a system of N spins with a certain number, say L, of spin pair interactions. This Hamiltonian is an appropriate model to describe magnetic phenomena. In the case of the spin-1/2 Ising model, it is given by [3,4]:

$$H = -J \sum_{\langle ij \rangle}^{L} \sigma_i \sigma_j - mh \sum_{i}^{N} \sigma_i , \tag{1}$$

where J is the spin-spin interaction strength (coupling constant), m the magnetic moment of the spins and h a magnetic field that acts along the z direction. It is understood in eq. (1) that the spin interaction is only due to the z components. In this sense, H is a one-dimensional Hamiltonian in the space of spin. Nonetheless, in general it is a d-dimensional Hamiltonian in real space ($d \leqslant 3$). This latter fact is fixed by the type of lattice in which the spins are located. The first sum in eq. (1) takes this detail into account: it runs over all L nearest-neighbor pairs of spins in the lattice. The second sum is simply over all spins, and it describes their independent interaction with the field. The magnitudes σ_i take only the values ± 1, and they describe the spin up and spin down states.

The knowledge of the Hamiltonian allows one to compute, at least formally, the partition function Z [3,4,12]

$$Z = \operatorname{tr} \exp(-\beta H); \quad \beta = 1/kT, \tag{2}$$

where, as usual, k is the Boltzmann constant and T the absolute temperature. The evaluation of all thermodynamic functions is in principle straightforward from eq. (2). Let us consider three of them, which are important to our later discussion: the spontaneous magnetization M_0, the magnetic susceptibility χ_0, and the specific heat at constant field C_h, all of them at zero-field intensity ($h \to 0$). Their expressions are as follows [3,4,12]:

$$M_0 = (1/\beta)\, \partial \ln Z / \partial h \,|_{h=0} = m \sum_i \langle \sigma_i \rangle |_{h=0} , \tag{3a}$$

$$\chi_0 = (1/\beta)\, \partial^2 \ln Z/\partial^2 h\,|_{h=0} = m^2 \beta \sum_i \sum_j \langle \sigma_i \rangle |_{h=0} \,, \tag{3b}$$

$$C_h = k\beta^2\, \partial^2 \ln Z/\partial^2 \beta\,|_{h=0}, \tag{3c}$$

where $\langle \ldots \rangle$ denotes the statistical expectation value.

The occurrence of a *phase transition* is represented by the occurrence of a *physical singularity,* whose *location* is the same for *all thermodynamic functions.* Here, we understand by "physical singularity" the existence of a real and positive temperature T_c (critical or transition point) where the singularity is located. If f represents any of the above thermodynamic functions, its asymptotic behavior near the critical point T_c can be expressed as follows:

$$f \approx A^{(f)}(T)\,(1 - T/T_c)^{a(f)} + \text{const}, \qquad T < T_c\,, \tag{4a}$$

$$f \approx A'^{(f)}(T)\,(1 - T_c/T)^{a'(f)} + \text{const}, \qquad T > T_c\,. \tag{4b}$$

Equations (4) may correspond to branch points or poles in the real T semi-axis.

The constants appearing in eqs. (4) are the critical parameters, and they are the most important constants in the theory of critical phenomena. The exponents a and a' are known as critical exponents, and $A^{(f)}(T_c)$, $A'^{(f)}(T_c)$ are the critical amplitudes.

Even though the location of the singularities is the same for all functions f, in general this is not the case for the critical exponents and amplitudes. Nevertheless, several conjectured relationships are supposed to be valid for them [2,3,13]:

(i) Universality hypothesis: $a(f)$ are only dependent on the dimensionality of the lattice, i.e. they do not depend on its structure.

(ii) Symmetry hypothesis: $a'(f) = a(f)$.

(iii) Scaling (and hyperscaling) hypothesis: some relationships are satisfied among several critical exponents and the dimension of the lattice, i.e. not all of them are independent.

It is clear that the verification of these and other hypotheses requires the accurate determination of the critical exponents.

In certain cases, the computation of critical parameters, which we discuss below, becomes a difficult task due to the fact that $T = T_c$ may not be the closest singularity to the origin. For example, the function $A^{(f)}(T)$ might possess singularities for complex values of T, whose moduli are smaller than T_c. These are *nonphysical* singularities, but they are important because they interfere in the location of the physical ones [3]. Studies have been carried out in the past about these interfering singularities on Ising models [13–17], as well as Heisenberg [18] and $X-Y$ models [19].

The nonphysical singularities possess their own characteristic critical exponents and amplitudes. However, as they are not located on the real T axis, their determination requires the use of different techniques. In this paper, we are concerned essentially with this problem.

Two different approaches have been developed to determine the critical parameters characterizing the singular points: the analysis of power series expansions and the renormalization group theory [3,4,13]. These methods lead to independent results.

The method based on power series expansions is easily justifiable and it has been extensively used. Its essential purpose is to express $\ln Z$ as a series in powers of some function of temperature. Several procedures have been developed to obtain such expressions, and the use of graph-theoretical techniques has shown to be valuable in computing the contributions of many-body interactions [3,4]. These expansions are, of course, the equivalent to the virial series in the theory of fluids.

After applying this method, we obtain a Taylor series representation of the thermodynamic functions [eqs. (3)]. Consequently, the critical parameters have to be determined only from a finite number of Taylor coefficients, and a number of methods are available to that purpose [3,4].

The RGT is based, on the other hand, on speculative, though reasonable, physical suppositions [4,13,20,21]. This theory predicts several scaling relationships among critical exponents. However, it is difficult to verify them numerically within the context of the theory. Due to this, a large comparative study of this method and the procedure based on power series expansions has been carried out in order to test the RGT conclusions.

High- and low-temperature (with reference to the physical critical point T_c) series (HTS and LTS, respectively) have been widely used in studying magnetic phase transitions in spin-lattice models. The HTS are most often taken into consideration, because the singularity pattern is simpler in that temperature range [3]. Owing to this, a number of methods that are successful when dealing with HTS [3,4] do not apply to LTS. This is mainly due to the fact that the convergence radius of the LTS is frequently determined by the above mentioned nonphysical (i.e. non-real) singular points [3,14–17]. However, valuable information is obtained from both series. As a matter of fact, the comparison of the critical behavior of functions given by eqs. (3) when approaching from the left and from the right to T_c enables one to test the RGT results (such as the symmetry hypothesis). Although the physical singular point at T_c is the one that really matters, it is often useful to calculate those that determine the LTS convergence radius. Even an approximate determination of these singular points often allows one to improve the computation of the physical singularity [18,19].

One of the purposes of the present paper is to obtain the critical parameters characterizing the singular points of the thermodynamic functions in the range of temperatures smaller than T_c. To this end, an alternative method is developed in sect. 2 and applied to a simple test example. The LTS for two spin-1/2 Ising models, namely, the three-dimensional face-centred cubic and body-centred cubic lattices, are considered in sect. 3. A strategy is suggested for the determination of the critical parameters characterizing all interfering singularities, without previous estimation of the physical singularity. Even though we are mostly concerned with the study of spin-lattice models, we show that the present method applies to a large class of different problems. Conclusions are found in sect. 4.

2. The method

Let $f(z)$ be a function of the complex variable $z = x + iy$ with the following properties: $f(z)$ is analytic at $z = 0$ and $f(x)$ is real. Therefore, every singular point of $f(z)$ is either a real or complex conjugate of another one and all the coefficients of the Taylor series,

$$f(z) = \sum_{n=0}^{\infty} f_n z^n, \tag{5}$$

are real. We are interested in the case where the convergence radius of (5) is determined by a pair of complex conjugate singular points, say $z_0 = x_0 + iy_0$ and $z_0^\star = x_0 - iy_0$. The moduli of the other singularities of $f(z)$ are supposed to be larger than $|z_0|$ and the form of $f(z)$ close enough to z_0 or $z_0^\star$ is assumed to be approximately given by:

$$f(z) \approx F_0 + A(z^2 - 2x_0 z + x_0^2 + y_0^2)^a, \tag{6}$$

where F_0 and A are, in general, complex numbers and a is real.

It is our purpose to develop a method for obtaining the critical parameters x_0, y_0 (critical point), a (critical exponent), and A (critical amplitude), which characterize the singular points at z_0 and $z_0^\star$, from the power series (5). The procedure is quite general and applies to all sorts of singularities (algebraic, exponential, and logarithmic [22]), but is enough for our present aims of considering only the above case. Others are treated similarly, as shown in sect. 3. In the particular case of algebraic singularities, the asymptotic form given by eq. (6) would be equivalent to representing $f(z)$ by a truncated expansion about a branch point or pole [22,23]: $f(z) \approx F_0 + F_1(z - z_0)^a$. In this latter instance, we would find: $A = F_1/(z_0 - z_0^\star)^a$ [cf. eq. (6)] [23].

The asymptotic form of the Taylor coefficients f_n is certainly determined by the singular points at z_0 and $z_0^\star$. Therefore, it is expected that the large-n behavior of f_n will equal that of the Taylor coefficients for the function in eq. (6). A similar assumption is also the basis of the widely accepted ratio method [3].

In order to calculate the critical parameters, we define the generating function (from now on, our procedure will be called generating function method, GFM)

$$Y(z) = B(z^2 - 2wz + r^2)^b, \tag{7}$$

where B, w, r^2, and b are adjustable real parameters. The Taylor coefficients of $Y(z)$ obey the following recursion relationship

$$(n-2b-1)\,Y_{n-1} + 2w(b-n)\,Y_n + (n+1)r^2\,Y_{n+1} = 0\,, \tag{8}$$

where $Y_0 = Br^{2b}$ and $Y_n = 0$ if $n < 0$. As argued before, it is expected that the Taylor coefficients f_n satisfy (8) for large enough n values provided $b = a$, $w = x_0$, and $r^2 = x_0^2 + y_0^2$. Therefore, to obtain the actual critical parameters we merely replace Y_j by f_j in eq. (8) for $n = N$, $N+1$, and $N+2$, and then solve for b, w, and r^2. The sequences b_N, w_N, and r_N^2 so obtained must converge towards a, x_0, and $x_0^2 + y_0^2$, respectively, as N tends to infinity. The GFM reminds one of the "n-point fit method" [3,17] (related to the Padé approximants), but they are not equal. The latter makes use of a different linearization procedure, and its applications have explicitly taken into account the singular points outside the convergence circle. On the other hand, the GFM requires only the knowledge of the form of $f(z)$ near the closest singularity to the origin, and even this information can be obtained by trial and error.

A straightforward algebraic manipulation shows that the GFM sequences are given by [23]:

$$w_N = \Delta(W_N/U_N)/\Delta(V_N/U_N)\,, \tag{9a}$$

$$r_N^2 = \Delta(W_N/V_N)/\Delta(U_N/V_N)\,, \tag{9b}$$

$$\begin{aligned} b_N = {} & [2w_N Q_N\,\{(N+1)^2 Q_{N+1}/(N+2)Q_{N+2} - N\} \\ & + N(N+1)\,Q_N/(N+2)\,Q_{N+2} + N - 1]\,/\,[2 - 2(N+1)\,Q_N/(N+2)\,Q_{N+2} \\ & + 2w_N Q_N\,\{(N+1)\,Q_{N+1}/(N+2)\,Q_{N+2} - 1\}]\,, \end{aligned} \tag{9c}$$

where $U_N = 2(b_N - N)$, $V_N = (N+1)Q_N$, $W_N = (2b_N - N + 1)/Q_N$, $Q_N = f_N/f_{N-1}$, and $\Delta P_N = P_{N+1} - P_N$. Upon substituting (9a) into (9c), we obtain a quadratic equation for b_N with only one acceptable root (the other one leads either to a divergent b_N sequence or to negative r_N^2 values).

The method is flexible and enables one to profit from available useful information about the problem function. For example, if the value of the parameter a is known beforehand, we can simply use eqs. (9a) and (9c) with $b_N = a$. This certainly improves the results and has recently proved to be useful in dealing with the perturbation series for some periodic eigenvalue problems [23]. Besides, it is a well-known fact that the critical point can always be much more accurately calculated than the critical exponent. We can therefore make use of a previous estimate of the former and calculate the latter through eq. (9c). This may be advantageous, as shown later.

The critical amplitude A can also be calculated provided it is real. Since $Y_n(w, r^2, b, B) = B Y_n(w, r^2, b, 1)$, the sequence

$$B_N = f_N / Y_N(w_N, r_N^2, b_N, 1)\,, \tag{10}$$

is believed to converge towards A as N increases. When A is not real, then B_N is found to be oscillatory.

Let us illustrate the above ideas with a test example. Consider, for instance, the following implicit equation:

$$z^2 + z = f(z) \exp\{f(z) + 1\}\,, \tag{11}$$

that defines a function $f(z)$ with the required properties. In fact, $f(z)$ has a pair of conjugate branch points of order one [22], given by the roots of $\mathrm{d}z/\mathrm{d}f = 0$. It can easily be shown that in a small vicinity of either $z_0 = (-1 + 3^{1/2}\mathrm{i})/2$ or $z_0^\star$, the function $f(z)$ behaves approximately as

$$f(z) \approx -1 + 2^{1/2}(1 + z + z^2)^{1/2}. \tag{12}$$

This example is non-trivial in the sense that the Taylor coefficients f_n do not reach the asymptotic form for finite n values. In addition, a very large number of Taylor coefficients can be easily calculated, which enables one to test the convergence of the GFM sequences.

Table 1 shows that the GFM sequences approach the actual critical parameters in a stepwise manner, due to which direct extrapolation is not advisable. It is preferable to deal with the three subsequences with subscripts $n + 3j$, $j = 0, 1, 2, \ldots$, where $n = m$, $m + 1$, $m + 2$, that are much smoother. After extrapolating them versus $1/j$ and averaging the three limits for each critical parameter sequence, we obtain $a = 0.4999 \pm 10^{-4}$, $x_0 = -0.50000 \pm 10^{-5}$, $|z_0| = 1.00000 \pm 10^{-5}$, and $A^2 = 1.99 \pm 0.02$, which closely agree with the actual values.

The high accuracy obtained in this case is certainly due to the fact that a very large number of Taylor coefficients have been used. In most physical applications, we will not be so fortunate and much less accurate results are to be expected. The most important fact is that this numerical example and many others not shown here (see ref. [23]) suggest that the GFM sequences are always convergent provided that the appropriate generating function is chosen.

Table 1

Critical parameter sequences for the function $f(z)$ defined by eq. (11)

N	$-w_N$	r_N	b_N	B_N
292	0.500004726	1.00001754	0.492582	1.35999
293	0.499998743	1.00000562	0.496018	1.38407
294	0.499982032	0.99997242	0.505647	1.44280
295	0.500004630	1.00001718	0.492658	1.36043
296	0.499998768	1.00000550	0.496059	1.38432
297	0.499982402	0.99997299	0.505587	1.44257
298	0.500004536	1.00001683	0.492732	1.36085
299	0.499998793	1.00000539	0.496098	1.38456
300	0.499982760	0.99997354	0.505529	1.44235

3. Spin-1/2 Ising models

The spontaneous magnetization M_0, the magnetic susceptibility χ_0, and the specific heat C_h in the zero-field limit [see eqs. (3)] for the spin-1/2 Ising models can be expanded in powers of $u = \exp(-4J/kT)$, where J is the spin-spin interaction [cf. eq. (1)]. A quite large number of Taylor coefficients are available for the *fcc* and *bcc* lattices (ref. [3], ch. 6), which we discuss as illustrative examples in this paper.

As mentioned before, the critical point is the same for all thermodynamic functions, but the critical exponents $a(M_0)$, $a(\chi_0)$, and $a(C_h)$ [eqs. (4)] are different.

Our purpose in this section is to discuss a possible strategy to determine the closest singularities to the origin in the thermodynamic function, using the method discussed in sect. 2. Our aim is to analyze how well these singularities can be located without using a biased input for the physical singular points. The proposed procedure has the advantage of allowing one to focus attention only on a restricted set of Taylor coefficients. By only considering those of largest order (i.e. those fixing the asymptotic behavior), one might find a best approximation to the dominating, nonphysical singularities. On the other hand, direct, unbiased application of Padé-like methods requires the use of *all* Taylor coefficients to end up with a not very reliable simultaneous approximation to all branch points and poles.

One would like to determine in the first place these interfering singular points. Proceeding this way, it is possible to factorize them from the original function and then to accomplish the study of the physical singularities. Another alternative method would be to use a conformal mapping to map the dominating (nonphysical) branch points outside the convergence disk [3,18,19]. Several procedures are available to perform this transformation, and we think that the present method could serve as a complementary tool.

Let us start with the critical exponent sequences for the above mentioned thermodynamic functions corresponding to the *bcc* lattice. First, we try to determine which function is more appropriate to accomplish the analysis. In other words, we determine for which function the sequences associated to the nonphysical singularities are smoother.

We find that, in general, all the sequences for $a(M_0)$, $a(\chi_0)$, and $a(C_h)$ are strongly oscillatory, and with no clear trend. This is a common characteristic of functions possessing a strong interference of singularities, and it has already been found even when using procedures based on a previous factorization of the physical singularity [3,14–17]. However, we notice that the oscillation in the sequences is not the same for all thermodynamic functions. For instance, upon averaging the results for the last five terms ($23 \leqslant N \leqslant 27$), we find: $b(C_h) = -1.0 \pm 0.6$, $b(M_0) = 0.4 \pm 2.5$, and $b(\chi_0) = -0.4 \pm 4.2$. It is clear that no reliable estimation can be obtained for the critical exponents of the spontaneous magnetization and magnetic susceptibility using this first simple approach. Nevertheless, a crude first estimation of the exponent corresponding to the specific heat can be made.

It is worth commenting that this result shows that the GFM provides an approximation different to that obtained when using other techniques, which provide the least accurate results for $a(M_0)$ and $a(C_h)$. This fact can be explained as follows: the most reliable calculations suggest that $a(C_h)$ is larger than $\alpha' \approx 1/8$, $a(\chi_0)$ is similar to $\gamma' \approx 21/16$, and $a(M_0)$ is smaller than $\beta \approx 5/16$, where α', γ', and β are the respective critical exponents of the *physical* singular point. Therefore, the physical singularity is somewhat dominant in M_0 and the methods that factorize it are more successful in calculating $a(M_0)$ than in calculating either $a(\chi_0)$ or $a(C_h)$. On the other hand, we try to obtain the critical parameters of the nonphysical singularities directly, and for this reason we find it easier to deal with the LTS for C_h that is dominated by those singular points.

As discussed above, we start our analysis with the specific heat power series. Of course, our aim is to obtain the critical parameters characterizing all three thermodynamic functions. To that end, we propose to pursue the following strategy to study different lattices:

(i) determine the approximate location of the pair of dominating complex singularities of the *bcc* lattice, using the C_h LTS;

(ii) obtain error bounds for the (nonphysical) critical exponents of other thermodynamic functions from the range of b values where the location of the singularity remains within the interval found in (i);

(iii) if a lattice possesses *more than* two complex interfering singularities, start the analysis again with the C_h LTS but considering the critical exponent of the *bcc* lattice transferable (extension of the symmetry hypothesis).

In what follows, we discuss an application of the above procedure to two spin-1/2 Ising models.

As mentioned above, we found a first estimation $a(C_h) \approx b(C_h) = -1.0 \pm 0.6$ for the *bcc* lattice. In the same way, the sequences w_N and r_N^2 for C_h, which are considerably smoother, lead to the following estimates (see table 2):

$$x_0 \approx -0.233 \pm 0.007, \quad y_0 \approx 0.304 \pm 0.009, \tag{13}$$

which agree with $x_0 \approx -0.234 \pm 0.001$ and $y_0 \approx 0.306 \pm 0.002$ obtained through the Padé approximants built from the factorized LTS for M_0 [3,15,16]. It is worth mentioning that, in order to derive this latter result, a first estimation of the physical critical parameters is necessary, and to transfer them from M_0 to C_h. We will use this result, together with (13), to provide the input data to develop the above mentioned strategy.

Table 2

Sequences for the location of the nonphysical singularities of the spin-1/2 Ising model on a *bcc* lattice. (Results using the LTS expansions for the specific heat capacity.)

N	$-x_0$	y_0
23	0.24177	0.31544
24	0.22624	0.29526
25	0.22629	0.29532
26	0.23709	0.30887
27	0.23262	0.30289

Estimates: $x_0 = -0.233 \pm 0.007$ $y_0 = 0.304 \pm 0.009$

A first rough estimate of the exponents $a(M_0)$ and $a(\chi_0)$ can be performed from the result (13). Let us consider, for instance, the largest term ($N = 27$) in the series expansions for the spontaneous magnetization. The parameter w_{27} (or $[(r_{27})^2 - (w_{27})^2]^{1/2}$) can be seen as a function of the approximate exponent $b_{27}(M_0)$. Therefore, a reasonable confidence interval for the latter can be obtained under the constraint that w_{27} will take only values within the interval given by the equalities (13). Proceeding this way, we find $a(M_0) \approx -0.15 \pm 0.75$. A similar reasoning leads us to $a(\chi_0) \approx -1.05 \pm 0.75$ for the magnetic susceptibility. It is clear that these results are not outstanding in accuracy; however, they represent a large improvement with respect to the previous estimates from the sequences, and they suggest a procedure to provide even better ones.

Bearing in mind the previous analysis, we proceeded to improve our results *by determining the largest and smallest b value giving rise to critical-point sequences whose last ten terms agree, within the error bounds, with the estimates given above.* We have performed the computations with the estimates (13) and with the more accurate ones given in refs. [3,15,16]. The results do not show significant differences, even though the confidence intervals are obviously somewhat tighter in the second case. Furthermore, when the latter results for x_0 and y_0 are used, one can also improve the estimate of exponent $a(C_h)$. Following the above procedure, we thus obtain: $a(C_h) \approx -1.12 \pm 0.02$, $a(M_0) \approx -0.11 \pm 0.03$, $a(\chi_0) \approx -1.10 \pm 0.02$, that appear to be more accurate than those reported previously [3,14–17].

According to the strategy already discussed, one may use the critical parameters obtained from the *bcc* lattice to study a different one, for instance the *fcc* lattice. This is consistent with the universality hypothesis, supported by extensive numerical evidence. In our particular case, *we will use the bcc critical exponents computed before in calculating the critical point for the fcc lattice.*

When one uses the generating function (7) with $b = a$ for the *fcc* lattice, the sequences are found to be wildly oscillatory. This represents a distinguishing feature between the two models. This behavior cannot have any relation with the transference of critical exponents between both lattices, which is in fact our main supposition. Accordingly, it should be due to the effect of *some other interfering singular points.* In other words, the generating function must be improved in order to describe the model properly. The method presented in sect. 2 can be immediately adapted to this new situation, as shown below.

The critical exponents of different singularities are not expected to be equal [3,15,16]. However, since the estimation of the critical point does not depend too strongly on the chosen critical exponent, we can try, in first approximation, the following generating function:

$$Y(z) = B(c_0 + c_1 z + c_2 z^2 + c_3 z^3 + z^4)^a \, . \tag{14}$$

Its Taylor coefficients satisfy the relation:

$$(n+1)c_0 Y_{n+1} + (n-a)c_1 Y_n + (n-2a-1)c_2 Y_{n-1} + (n-3a-2)c_3 Y_{n-2}$$
$$+ (n-4a-3) Y_{n-3} = 0 \, . \tag{15}$$

Upon solving all the sets of four linear equations generated by (15), with $Y_j = f_j$ and $n = N$, $N+1$, $N+2$, and $N+3$, we obtain the sequences $c_m^{(N)}$, $m = 0, 1, 2,$ and 3, $N = 3, 4, \ldots$. Once again, those for C_h (displayed in table 3) are found to be the smoothest ones. By averaging the last ten results obtained with $a = -1.14$ and $a = -1.10$ (*vide supra*), we estimate: $c_0 \approx 0.0803 \pm 0.0003$, $c_1 \approx 0.218 \pm 0.001$, $c_2 \approx 0.436 \pm 0.002$, and $c_3 \approx 0.746 \pm 0.002$. The singular points, given by the four roots of $Y(z) = 0$, are found to be z_0, $z_0^\star$, z_1, and $z_1^\star$, where:

Table 3

Location of dominating singularities of the spin-1/2 Ising model on an *fcc* lattice: sequences for the coefficients c_i of eq. (14) from the C_h LTS. (Results for $a = -1.12$)

N	$c_0^{(N)}$	$c_1^{(N)}$	$c_2^{(N)}$	$c_3^{(N)}$
30	0.080450	0.21852	0.43918	0.75647
31	0.078816	0.21350	0.42970	0.73766
32	0.081070	0.21712	0.43435	0.74435
33	0.080325	0.21822	0.43533	0.74390
34	0.080377	0.21730	0.43718	0.74578
35	0.080168	0.21681	0.43477	0.74640
36	0.080098	0.21632	0.43369	0.74233
37	0.080605	0.21758	0.43568	0.74535
38	0.080248	0.21736	0.43560	0.74497
39	0.080289	0.21700	0.43553	0.74524
40	0.080260	0.21698	0.43887	0.74487

$$z_0 \approx \{-0.4465 \pm 0.0015\} + \{0.279 \pm 0.005\}\mathrm{i}\,, \tag{16a}$$

$$z_1 \approx \{-0.0733 \pm 0.0006\} + \{0.533 \pm 0.001\}\mathrm{i}\,. \tag{16b}$$

The two pairs of conjugate singularities interfere very strongly because $|z_0| = 0.527 \pm 0.003$ is very close to $|z_1| = 0.538 \pm 0.001$. Present results seem to be somewhat more accurate than those reported previously [3,15–17], which in some cases take into account two different exponents [15,16]. This fact confirms our assumption that the choice of the critical exponent has no strong effect on the estimated critical point, and that in fact it can be transferred between different lattices, disregarding the number of dominating singularities. It is supposed that a more elaborate generating function could lead to more accurate results.

The present estimates of the critical parameters for the nonphysical singularities in the spin-1/2 Ising models on lattices *bcc* and *fcc* can be used to improve the results for the physical singularities. As commented before, a conformal mapping can be used to map present singularities outside the convergence disk (see, for example, the method in refs. [18,19]).

4. Further comments and conclusions

A method for obtaining critical parameters from power series expansions has been presented. Although examples with complex conjugate singular points nearest to the origin only have been treated here, it is clear that the GFM can be applied to a larger class of problems. For instance, the generating function $B(1 - z/w)^b$ proves to be useful when the convergence is determined by an isolated real singularity, in which case the ratio method equations [3] are obtained. In addition, the generating functions discussed in sect. 3 are also suitable when there are real singular points.

Both the Padé approximants [3,15,16] and the GFM are general and in some cases they appear to be complementary. In fact, it has been shown in sect. 3 that while the Padé approximants yield the most accurate results for M_0, the GFM is most appropriate to deal with the C_h LTS. Furthermore, they provide independent results because the GFM is always applied without previous factorization of the physical critical point. As a conclusion, we deem that the method and strategy discussed in this paper to study spin-lattice models might be valuable in obtaining a more reliable set of critical parameters. Moreover, it may also be used to check the validity of the confidence intervals estimated for these parameters.

Finally, present and previous numerical investigations [23] suggest that the GFM can be fruitful as a tool in series analysis.

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