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2002 J. Phys. A: Math. Gen. 35 4429

(http://iopscience.iop.org/0305-4470/35/20/304)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 4429–4441 PII: S0305-4470(02)32676-3

Improved methods of estimating critical indices via fractional calculus

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Received 10 January 2002, in final form 11 April 2002
Published 10 May 2002
Online at stacks.iop.org/JPhysA/35/4429

Abstract
Efficiencies of certain methods for the determination of critical indices from power-series expansions are shown to be considerably improved by a suitable implementation of fractional differentiation. In the context of the ratio method (RM), kinship of the modified strategy with the *ad hoc* 'shifted' RM is established and the advantages are demonstrated. Further, in the course of the estimation of critical points, significant betterment of convergence properties of diagonal Padé approximants is observed on several occasions by invoking this concept. Test calculations are performed on (i) various Ising spin-$1/2$ lattice models for susceptibility series attended with a ferromagnetic phase transition, (ii) complex model situations involving confluent and antiferromagnetic singularities and (iii) the chain-generating functions for self-avoiding walks on triangular, square and simple cubic lattices.

PACS numbers: 02.30.Sa, 05.70.Jk, 75.40.Cx

1. Introduction

Given the first few (up to $n = N$) coefficients f_n of a power-series representation of some function $F(x)$ in the form

$$F(x) = \sum_{n=0} f_n x^n, \tag{1}$$

it is often [1–10] of interest to estimate the radius of convergence (X) and examine the nature of singularities in $F(x)$. Important situations in chemical physics involve the virial series and studies on condensation [1, 2], self-avoiding walks [3, 4] and the susceptibility series for various lattice models exhibiting magnetic phase transitions [4–10]. Determination of critical

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0305-4470/02/204429+13$30.00

indices, e.g. the critical point X and the critical exponent λ, on the basis of an assumed, but widely accepted, form for $F(x)$:

$$F(x) \cong A\left(1 - \frac{x}{X}\right)^{\lambda} \tag{2}$$

as $|x| \to X$, has thus emerged as an active area of research over recent decades. In (2), A is the critical amplitude, the exponent λ is usually a non-integer and satisfies $\lambda < 0$, and X defines the dominant singularity closest to the origin. Various methods are available to tackle the problem (see, e.g., [4,5] and references therein). However, we shall be concerned here with two simple strategies. One of these is the ratio method (RM) [6]. It is perhaps the simplest, oldest and the most favoured tool. On its own, however, the scheme performs fairly well. Coupled with a sequence accelerator, the RM can offer more satisfactory results [4, 5]. In complex situations, undesirable singularities in $F(x)$ are mapped away, before employing the RM, by using a change of variable at the onset; refinements were subsequently made [7, 8] in other respects too. Of these, one specific variant, the shifted RM (SRM) [5, 8], rests on the *ad hoc* introduction of a parameter s that is either arbitrarily held fixed (at $s = 0.5$) to improve the convergence of the values sought [5], or optimized [8]. The SRM possesses an edge over other ratio-type methods in that it retains the essential simplicity of the RM. We now turn our attention to the other strategy, which is based on Padé approximants (PA) [11]. The PA have been employed in various ways [4, 5, 9] to tackle the problem to hand. Here we choose a simple route. From (1), if we define ratios $R_n = f_n/f_{n-1}$, the sequence of values of R_n would approach a limit R_∞ and X may be defined as $X = 1/R_\infty$. Sequences of diagonal PA (DPA) of a given parent sequence are known to converge much better [11, 12] on several occasions. Therefore, we expect better estimates of R_∞, and hence of X, by forming such DPA sequences. A 'biased' scheme [4] may subsequently be adopted to find λ.

From (1) and (2), we notice that, if $F(x)$ is k-times differentiated, the position of the singularity does not change. The alterations in λ and A are also known. So, one may be tempted to explore whether the use of such $D^k F(x)$ series ($k = 1, 2, \ldots$) are beneficial in providing nicer estimates of X, λ and A. One disadvantage is, however, immediate. The known number of coefficients decreases from N to $(N - k)$. Therefore, *a posteriori* application of some convergence accelerator [4, 5, 9, 11–13] would be generally less profitable. As we shall see presently, one can avoid the difficulty by invoking the concept of fractional differentiation [14–18]. It has two advantages: it does *not* reduce the number of terms; moreover, an extra parameter k is embedded in a technique that can be chosen profitably. Fractional calculus (see [18] for a recent review) has so far been employed in areas such as electrochemistry [14], diffusion [15] and scaling in phase-transition processes to generalize [16] Ehrenfest's classification. Our endeavour highlights a new area of application of the same.

The aim of the present paper is threefold. First, we show how to incorporate a parameter in the RM through fractional calculus in a *natural* way that considerably improves the efficiency of the scheme, but not at the cost of simplicity. We henceforth call it the fractional RM (FRM). Next, we establish a close kinship of the FRM with the prevalent SRM and demonstrate their comparative performance. For brevity, we do not employ here any sequence accelerator. This is because our purpose in hand is not to extract highly accurate values of X or λ; rather, we would like to stress the properties and efficiency of the FRM. Finally, we demonstrate that fractional differentiation of (1) may often provide superior estimates of X through the DPA. This strategy is referred to here as the fractional DPA (FDPA). The FDPA reveals yet another practical advantage of the calculus.

2. The scheme

Here, we first briefly survey the salient features of the RM and the SRM, and then proceed to introduce the FRM and the FDPA. Note that, if (2) holds strictly, then one can write

$$F(x) = A \sum_{n=0} \binom{\lambda}{n} (-1/X)^n x^n, \tag{3}$$

where the binomial coefficient is to be evaluated by using a Γ function for non-integral λ. Let us mention at this point that we shall consider here both an unbiased scheme such as the RM, the SRM or the FRM, and part of a biased scheme such as the DPA or the FDPA. In an unbiased scheme, one evaluates the unknown quantities such as X and λ independently. In a biased approach, in contrast, employing an assumed or known value for X, the sequence for λ, for example, is constructed. Specifically, we shall explore how a better value of X can be found from the ratios. So, part of our concern remains unbiased.

2.1. The RM and the SRM

From the definition of R_n, coupled with (3), it follows that

$$R_n = \frac{1}{X}\left(1 - \frac{\lambda + 1}{n}\right). \tag{4}$$

Taking two different n values, we can solve (4) to get X and λ. Now, n can be varied to generate two different sequences of estimates for X and λ. For close-packed lattices, it is customary to choose consecutive n values, while the odd and even R_n sequences are first separated for loose-packed lattices, before solving (4). This strategy is known as the RM. The situation in most cases, however, is not so simple. Higher-order terms in $1/n$ are indeed present within the parentheses of (4). A major reason is that (2) is an approximation for most practical purposes. Confluent singularities are often believed to be present. Then, $F(x)$ is given instead by

$$F(x) = \sum_{j=1} A_j \left(1 - \frac{x}{X}\right)^{\lambda_j}, \tag{5}$$

where $\lambda_1 < \lambda_2 < \lambda_3$, etc. These other subdominant singularities, defined by the exponents λ_2, λ_3, etc, affect the convergence of R_n, and hence of the sequences obtained for X and λ_1, when N is not large enough. A more general form for $F(x)$ is

$$F(x) = \sum_{j=1} A_j \left(1 - \frac{x}{X_j}\right)^{\lambda_j}. \tag{6}$$

Guttmann [4] discussed at length such types of complications. However, a special case of (6) deserves more attention [9]. It corresponds to an antiferromagnetic singularity, in addition to the ferromagnetic one that is being studied. In this situation, j in (6) runs up to 2 and $X_1 = -X_2$. It is characteristic of loose-packed lattices. Now, an important point is that the form (5) or (6) does not lead to (4). Even if one chooses a much simpler situation allowing merely a slow variation in the amplitude A, i.e.

$$F(x) = A(x)\left(1 - \frac{x}{X}\right)^{\lambda}, \tag{7}$$

where $A(x)$ can be expanded in the form $A(x) = A(X) + (x - X)A'(X) + \cdots$ as $|x| \to X$, one finds

$$R_n = \frac{1}{X}\left(1 - \frac{\lambda + 1}{n} + \mathrm{O}(1/n^2)\right). \tag{8}$$

In other words, a *series* in $1/n$ appears in the parentheses now. Therefore, the RM cannot converge rapidly. By introducing an *ad hoc* shift in n, the SRM tries to remedy the error. One writes

$$R_n = \frac{1}{X}\left(1 - \frac{\lambda + 1}{n + s}\right), \tag{9}$$

so that, on expansion ($s \ll n$), (9) becomes structurally similar to (8). Earlier [5], the parameter s was set fixed at 0.5. However, we can also solve (9) [8] for X and λ, by taking three successive R_n and n values. Specifically, one obtains

$$X = -\frac{\Delta^2 R_n}{R_{n+2}\Delta R_n - R_n \Delta R_{n+1}}; \qquad \lambda = \frac{(1 - XR_n)(1 - XR_{n+1})}{X\Delta R_n} - 1. \tag{10}$$

In (10), Δ is the standard forward difference operator, defined by $\Delta g(n) = g(n+1) - g(n)$, $g(n)$ being some function of n. One may obtain a value for s at each step as well, if one likes, though it is not necessary. The procedure is essentially the same as that of the RM, outlined below (4). However, it often yields much better results than the parent version.

2.2. The FRM

We define the fractional differentiation process by

$$D^p y^m = \frac{\Gamma(m+1)}{\Gamma(m+1-p)} y^{m-p}, \tag{11}$$

where p may be a *non-integer* now. This fractional operator in (11) corresponds to the Riemann–Liouville version [17, 18]. Based on such a prescription, we differentiate (2) p times to obtain

$$D^p F(x) = A'\left(1 - \frac{x}{X}\right)^{\lambda - p}. \tag{12}$$

Here, A' is the new amplitude. Applying the RM on this transformed form (12), we would find new ratios $R_n(p)$ described by

$$R_n(p) = \frac{1}{X}\left(1 - \frac{\lambda + 1 - p}{n}\right), \tag{13}$$

analogous to (4), but with a changed exponent. On the other hand, we find from (1) that

$$D^p F(x) = A \sum_{n=0} \binom{\lambda}{n} (-1/X)^n \frac{\Gamma(n+1)}{\Gamma(n+1-p)} x^{n-p}. \tag{14}$$

Direct calculation of the ratios following (14) gives

$$R_n(p) = R_n \frac{n}{n-p}. \tag{15}$$

We can now combine (13) and (15) to write

$$R_n = \frac{1}{X}\left(1 - \frac{\lambda + 1 - p}{n}\right)\frac{n-p}{n}. \tag{16}$$

This is the required FRM equation where the parameter p has been embedded in a natural way. As before, we take three successive R_n and n to solve for X and λ at each step. This leads to the following results:

$$X = \frac{2}{\Delta^2(n^2 R_n)}; \qquad \lambda = 2n - X\Delta(n^2 R_n). \tag{17}$$

Thus, one may avoid the estimation of p. However, if one wishes, a pair of values for p could be obtained at each step.

A few points regarding the FRM are now in order. First, it takes care of the $1/n^2$ term that was lacking in (4). Convergence is thus expected to be much better than for the RM. Secondly, for large n, the FRM becomes equivalent to the SRM. This is because terms of order $1/n^3$ and higher, present in the SRM, tend then to zero. Thirdly, a close look at (16) reveals that, if p_1 is a solution, $(\lambda + 1 - p_1)$ is another solution. Stated otherwise, there exist two p values, p_1 and p_2, each satisfying (16), where

$$p_1 + p_2 = \lambda + 1. \tag{18}$$

In (18), the quantities λ and X refer to solutions of (16) at a particular stage. The symmetry of (16) is indeed responsible for the emergence of these *two* possible solutions of p. For future convenience, we shall designate by p_1 the larger solution of (16), i.e. $p_1 > p_2$. The significance of the two solutions will concern us later too. Nevertheless, as we commented before, one can eliminate p while employing (16) on three successive R_n values, as (17) shows. Thus, it is ultimately not necessary to pay attention to possible values of p, unless the situation demands it.

2.3. The FDPA

Given a partial sequence $\{R_j\}$, there is a standard recipe [11, 12] to construct the DPA-transformed partial sequence $\{T_k\}$. The total number of terms in the latter case, however, is roughly halved. Let us suppose that k in $\{T_k\}$ runs from 1 to K. Then, one way to judge the convergence of any transformed sequence is provided by the quantity

$$\sum_{k=1}^{K} |T_K - T_k|.$$

A better convergence will imply a smaller value of the above sum, for a fixed K. In the present case we make two modifications. As stated before, the required result for X is actually given by the limit of the inverse of either sequence. So, after making the transformation, we take the inverse of each member and estimate the index of convergence through a quantity δ, given by

$$\delta = \sum_{k=1}^{K} |T_K^{-1} - T_k^{-1}|. \tag{19}$$

The second modification has its root in (15). Once the series (1) is p-times differentiated, the new ratios forming the parent sequence $\{R_n(p)\}$ are related to the old ones by (15) but the value of X does not change (see (12)). For a particular value of p, the DPA-transformed sequence of $\{R_n(p)\}$ can be obtained by following the standard route. These will likewise be called $\{T_k(p)\}$. Therefore, $T_k(p)$ is an FDPA transform of $\{R_n\}$. The estimate δ in (19) will now depend on p. This brings forth an advantage over the plain DPA transforms (at $p = 0$). One may vary p to minimize δ, thus obtaining the 'best' transformed sequence. Indeed, we shall see that this simple prescription improves the quality of X considerably in many situations. Further, unlike the FRM, one finds here a unique value of p. Finally, it is obvious that the s shift in the SRM cannot provide any benefit in such a context.

3. Results and discussion

We consider first the high-temperature reduced magnetic susceptibility series for a few Ising spin-1/2 lattice models. The variable x in (1) then stands for $\tanh(J/kT)$, where J is the spin–spin coupling constant, k is the Boltzmann constant and T refers to the absolute temperature.

Table 1. Adequacy of the RM, SRM and FRM in simulating the overall variation of R_n with n for the series F1 and F2 (see the text) via a fitting procedure.

Series	Method	X	λ	CC
F1	RM	0.263 862	−1.599 109	0.998 106
($N = 16$)	SRM	0.268 193	−1.762 178	0.999 985
				($s = 0.250$)
	FRM	0.267 895	−1.745 048	0.999 993
				($p_1 = 0.153$)
				($p_2 = -0.898$)
F2	RM	0.996 521	−1.204 758	0.998 920
($N = 20$)	SRM	0.999 852	−1.240 907	1.000 000
				($s = 0.179$)
	FRM	0.999 681	−1.238 101	1.000 000
				($p_1 = 0.100$)
				($p_2 = -0.338$)

We also choose two test series, considered earlier by Graves-Morris [9], which have close correspondences with the former ones. Coefficients f_n of expansion (1) up to $n = N$ are known for triangular, face-centred cubic (fcc), body-centred cubic (bcc) and simple cubic (sc) lattices [4]. The series for the triangular lattice is henceforth designated by F1, for convenience. Model 2 of [9] illustrates how the Curie point λ is affected by the presence of a *confluent* singularity. We designate this series by F2. It has the form (5) with j running up to 2, $A_1 = 1.0$, $A_2 = 0.1$, $X = 1.0$, $\lambda_1 = -1.25$ and $\lambda_2 = -0.75$. Series F3, on the other hand, refers to model 1 of the same work [9]. It reveals the role of an *antiferromagnetic* singularity, corresponding to the Néel point, on the critical indices of a ferromagnetic phase transition. The form of F3 is similar to (6), but with just two terms. Thus, in this case, one takes $A_1 = 1.0$, $A_2 = 0.5$, $X_1 = 1.0$, $X_2 = -1.0$, $\lambda_1 = -1.25$ and $\lambda_2 = -0.875$. As for a few other test cases, we next choose the chain-generating functions for self-avoiding walks on triangular [4], square [4] and sc [3] lattices. In such contexts, f_n in (1) stands for the number of n-step self-avoiding walks on a particular lattice.

Having discussed the series under investigation, we now proceed to study first the efficacy of the FRM and then the FDPA.

3.1. Fitting and the ratio-type methods

First, we note that equations (4), (9) and (16) refer respectively to the RM, the SRM and the FRM. They all try to reflect the variation of R_n with n. Therefore, we may examine how far these equations are adequate in describing the overall behaviour of R_n when *all* the terms are considered. Here, the series considered are simpler. We show the results of such a fitting in table 1. For F1, we take $N = 16$ and notice that the correlation coefficient (CC) is closest to unity in the case of the FRM. Taking $N = 20$ for the series F2, we find that the SRM and the FRM perform almost similarly. Exact values of X and λ are known in both cases: $X = 1/(2+\sqrt{3})$ and $\lambda = -7/3$ in the triangular lattice problem (F1); $X = 1.0$ and $\lambda = -1.25$ for F2. The derived estimates of these quantities, obtained via fitting, are, however, not quite satisfactory. A major reason behind this is, our fitting process has laid equal emphasis on all ratios, though it is known that initially these R_n values behave wildly [4]. They settle to reflect the proper behaviour of the singularity sought only after a sizable number of terms, depending on the problem to hand. Nevertheless, we note that outcomes of the SRM or the FRM are much better compared to the parent RM. This indirectly hints that (9) or (16) are much better suited in mimicking the variations of R_n with n. The worth of the present endeavour in highlighting the

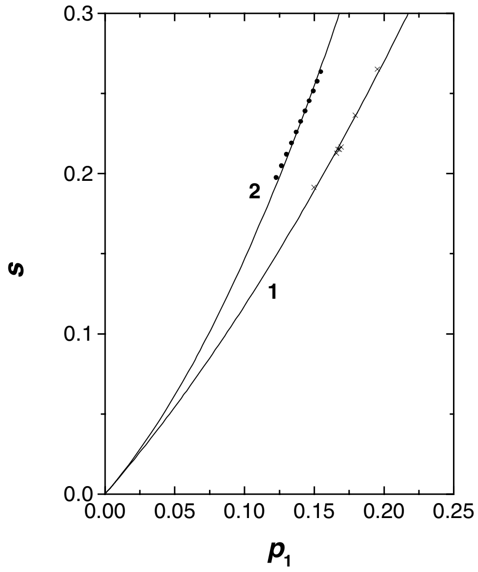

Figure 1. Plot of s versus p_1 (see text) showing the expected parabolic dependence. In the case of the triangular lattice referring to series F1 (curve 1), points are shown by crosses while circles refer to the series F2 (curve 2), both corresponding to the results presented in table 2.

efficiency of the FRM is thus partially justified. The table also shows the optimum values of s and p (p_1 and p_2). We find that s and p_1 are reasonably close, though n is not large enough.

3.2. *The role of the parameters in the SRM and the FRM*

We now explore any relation between s and p, the two essential parameters embedded in the modifications of the RM. To this end, we equate (9) and (16) for a particular n value with the assumption that X and λ are fixed quantities. This leads to the equation

$$p^2 - (\lambda + 1)p + \frac{(\lambda + 1)ns}{n + s} = 0. \tag{20}$$

A few interesting consequences of (20) are in order. First, we rediscover that the two roots of p, p_1 and p_2, satisfy (18). Second, the expression for the product $p_1 p_2$ yields, after a little rearrangement,

$$\frac{1}{s} = \frac{1}{p_1} + \frac{1}{p_2} - \frac{1}{n}. \tag{21}$$

It reveals that, at large n, s is really *half* the *harmonic mean* of p_1 and p_2. Third, in common situations, where $s > 0$ and $(\lambda + 1) < 0$, the larger root p_1 obeys $0 < p_1 < s$ if n is large. We thus see the role of s in providing a *bound* for p in the FRM. Finally, from (20), we also find that, in the large-n regime, the parameter s satisfies $s = p_1 p_2/(\lambda + 1)$. Coupled with (18), it implies that a plot of s versus p_1 would be parabolic in nature. In figure 1, we show such a plot for series F1 and F2. They correspond to the results to be found in table 2. Although n is never very large, we happily notice that the plots are essentially parabolic in both cases. It now remains to uncover the significance of the two roots p_1 and p_2. To this end, we take a simple function $(1 - x)^\lambda$. Then R_n is given exactly by $R_n = 1 - (\lambda + 1)/n$. Therefore, one finds $s = 0$ in the SRM; in other words, no shift is necessary here. By (20), we next find that $p_1 = 0$ and $p_2 = \lambda + 1$. The first solution clearly hints that one need not differentiate the series and

Table 2. Sequential estimates of X and λ by solving the RM, SRM and FRM equations for the series F1 and F2 (see text).

	X			λ		
N	RM	SRM	FRM	RM	SRM	FRM
(F1)						
10	0.267 468	0.267 875	0.267 866	−1.715 169	−1.745 489	−1.744 495
11	0.267 568	0.268 033	0.268 020	−1.719 180	−1.757 365	−1.755 823
12	0.267 636	0.267 982	0.267 974	−1.722 142	−1.753 178	−1.752 160
13	0.267 683	0.267 951	0.267 946	−1.724 409	−1.750 360	−1.749 651
14	0.267 721	0.267 948	0.267 944	−1.726 317	−1.750 055	−1.749 463
15	0.267 751	0.267 951	0.267 947	−1.727 979	−1.750 319	−1.749 797
16	0.267 776	0.267 952	0.267 949	−1.729 435	−1.750 476	−1.750 015
(F2)						
10	0.999 348	0.999 856	0.999 843	−1.231 604	−1.241 484	−1.241 148
11	0.999 442	0.999 875	0.999 865	−1.232 567	−1.241 856	−1.241 563
12	0.999 515	0.999 890	0.999 882	−1.233 392	−1.242 185	−1.241 925
13	0.999 574	0.999 902	0.999 896	−1.234 108	−1.242 479	−1.242 244
14	0.999 621	0.999 912	0.999 907	−1.234 739	−1.242 742	−1.242 529
15	0.999 661	0.999 921	0.999 916	−1.235 300	−1.242 980	−1.242 785
16	0.999 694	0.999 928	0.999 924	−1.235 802	−1.243 196	−1.243 017
17	0.999 721	0.999 935	0.999 931	−1.236 256	−1.243 394	−1.243 228
18	0.999 745	0.999 940	0.999 937	−1.236 669	−1.243 575	−1.243 420
19	0.999 766	0.999 945	0.999 942	−1.237 046	−1.243 743	−1.243 598
20	0.999 784	0.999 949	0.999 946	−1.237 393	−1.243 898	−1.243 761

should be satisfied with the RM results. The other solution, however, insists on a $(\lambda + 1)$-times differentiation. Once it is done, we obtain a series where the ratios *do not* depend on n at all. Thus, we extract the actual answer simply from the first ratio! Here lies the advantage of the second solution.

3.3. Comparative performance of the SRM and the FRM

We now turn our attention to sequential estimates of X and λ. This requires us to proceed through the strategy of *solving* equations like (10) and (17). For the RM, a similar pair of equations follows. In table 2, we display such results for the two cases, F1 and F2, discussed above. It is notable that the FRM yields results very close to those of the SRM in both cases. This conclusion applies to X as well as λ. These estimates, especially those of the exponents, are again much better in quality than what we get via the RM.

In table 3, we summarize the results found for other systems. In the fcc case, the scheme applies straightforwardly. However, antiferromagnetic singularities are present in sc, bcc and F3. So, the ratios oscillate and we first separate the odd and even ratios. Then, we employ the RM by taking two consecutive terms of the separated sequences. Likewise, the SRM and the FRM are applied by involving three such consecutive terms in each sequence. Here, only the last results are displayed. It is customary to apply a sequence accelerator to each (odd or even) such sequence of X or λ values and then take an average. However, here the estimates are simply averaged and yet we note that the average values (denoted by 'avg' in the table) are close to the actual ones [4, 8, 9] when the SRM or the FRM is employed. The two modified schemes again perform comparably. The advantage is clearer with estimates of λ.

Having realized that antiferromagnetic singularities affect more adversely [9] the estimation of the critical exponent, and that the initial oscillations of a series may lead to

Table 3. Critical indices for fcc, sc and bcc lattices, and the test series F3 (see text), obtained by adopting the different schemes. Except for the fcc case, final results are found after separating the even and odd terms. The average estimates (avg) are considered useful.

		X			λ		
N		RM	SRM	FRM	RM	SRM	FRM
(fcc)							
14		0.101 734	0.101 728	0.101 728	−1.246 767	−1.245 268	−1.245 261
(sc)							
	odd	0.218 303	0.218 147	0.218 140	−1.266 885	−1.249 834	−1.248 792
14	even	0.217 991	0.218 173	0.218 162	−1.233 050	−1.255 474	−1.253 725
	avg	0.218 147	0.218 160	0.218 151	−1.249 967	−1.252 654	−1.251 259
(bcc)							
	odd	0.156 222	0.156 106	0.156 101	−1.262 991	−1.245 325	−1.244 186
14	even	0.155 994	0.156 118	0.156 111	−1.228 414	−1.249 585	−1.247 990
	avg	0.156 108	0.156 112	0.156 106	−1.245 702	−1.247 455	−1.246 088
(F3)							
	odd	0.999 183	0.999 819	0.999 737	−1.093 222	−1.117 594	−1.113 248
20	even	1.000 829	1.000 256	1.000 237	−1.408 343	−1.386 631	−1.385 624
	avg	1.000 006	1.000 037	0.999 987	−1.250 783	−1.252 112	−1.249 436

Table 4. Variation of the average estimate of the critical exponent with N for the series F3 (see text) in different schemes.

	λ		
N	RM	SRM	FRM
10	−1.251 587	−1.272 893	−1.248 282
20	−1.250 783	−1.252 112	−1.249 436
30	−1.250 491	−1.251 144	−1.249 685
40	−1.250 352	−1.250 850	−1.249 786
50	−1.250 271	−1.250 712	−1.249 839
60	−1.250 219	−1.250 631	−1.249 872
70	−1.250 183	−1.250 577	−1.249 894
80	−1.250 156	−1.250 539	−1.249 910
90	−1.250 136	−1.250 510	−1.249 922
100	−1.250 120	−1.250 487	−1.249 931

unreliable answers [4] if N is not large enough, we now analyse the series F3 in greater detail. These results are succinctly presented in table 4. We notice that the average values follow a systematic trend in all cases. It is important to observe that the plain RM all along performs *better* than the SRM here. In addition, both the SRM and the RM approach the exact answer from *below*. On the other hand, the FRM works *best* even when N is not very large, and it tends to exactness from *above*.

We now consider the problem of self-avoiding walks. Table 5 displays results for the triangular lattice case. The D log PA method yields [4] closely: $X = 0.240\,88$ and $|\lambda| < 1.335$, on average. Our estimate of λ seems better in view of the discussion in [4]. In the case of a square lattice, results [4] of the D log PA again show that the average estimate of $|\lambda|$, ranging from 1.337 to 1.34, is lower than expected. Our data in table 6 reveal $|\lambda| > 1.3414$, implying that we are closer to the exact value of 1.343 75. The closeness is also true of X, though the improvement is marginal. We should also point out that the usual odd–even separation of the

Table 5. Critical indices for self-avoiding walks on a triangular lattice ($N = 20$). The table shows the last 10 results.

RM		SRM		FRM	
λ	X	λ	X	λ	X
−1.317 820	0.240 681	−1.301 855	0.240 499	−1.301 170	0.240 493
−1.320 162	0.240 731	−1.345 869	0.240 992	−1.344 310	0.240 980
−1.320 588	0.240 740	−1.325 470	0.240 786	−1.325 411	0.240 785
−1.321 481	0.240 756	−1.332 771	0.240 854	−1.332 464	0.240 852
−1.322 419	0.240 771	−1.335 309	0.240 876	−1.334 913	0.240 874
−1.323 184	0.240 783	−1.334 437	0.240 869	−1.334 136	0.240 868
−1.323 979	0.240 795	−1.336 519	0.240 885	−1.336 149	0.240 883
−1.324 707	0.240 805	−1.336 939	0.240 888	−1.336 588	0.240 886
−1.325 392	0.240 814	−1.337 606	0.240 892	−1.337 258	0.240 891
−1.326 038	0.240 822	−1.338 228	0.240 896	−1.337 883	0.240 895

Table 6. Critical parameters of series for self-avoiding walks on a square lattice ($N = 27$). The odd and even ratios are separately studied. The table shows the last 10 average results.

RM (avg)		SRM (avg)		FRM (avg)	
λ	X	λ	X	λ	X
−1.285 815	0.377 236	−1.535 342	0.380 975	−1.282 455	0.376 823
−1.305 585	0.378 280	−1.396 772	0.380 180	−1.358 312	0.379 548
−1.317 440	0.378 717	−1.408 145	0.380 027	−1.369 441	0.379 598
−1.321 338	0.378 820	−1.390 041	0.379 558	−1.346 395	0.379 142
−1.322 243	0.378 831	−1.362 164	0.379 177	−1.332 063	0.378 919
−1.323 611	0.378 859	−1.347 543	0.379 066	−1.335 618	0.378 975
−1.325 295	0.378 891	−1.348 997	0.379 090	−1.340 577	0.379 033
−1.326 711	0.378 916	−1.348 174	0.379 081	−1.340 980	0.379 037
−1.327 881	0.378 935	−1.346 503	0.379 067	−1.340 822	0.379 035
−1.328 921	0.378 950	−1.345 936	0.379 064	−1.341 393	0.379 040

ratios is done before applying any of the three schemes to the square lattice case. Table 6 shows the average results only, for brevity. The cubic lattice case has been discussed in detail [3] quite recently. Using differential approximants, which are known to be more powerful [4], it was found [3] that $X \approx 0.213\,494$ and $|\lambda| \approx 1.1605$. These results are slightly better than those we furnish in table 7. Here too, odd and even ratios are first separated and we display the average results only. The FRM is seen to provide the closest answers. Subsequent application of a sequence accelerative transform is likely to improve our results further towards the 'assumed' exact values [3], viz, $X = 0.213\,491$ and $|\lambda| \approx 1.1585$. In all the above cases, however, we have listed the last few results, avoiding insignificant fluctuations during the initial phase. The whole study makes it transparent that one gains a considerable advantage in most situations by adopting the SRM or the FRM, rather than the plain RM.

3.4. *Comparative performance of the DPA and the FDPA*

We finally focus attention on the FDPA. Here, we first choose a value of p, estimate $T_k(p)$ that are $[k/k]$ PA to the sequence $\{R_n(p)\}$ and then find δ via (19). The procedure is continued for various values of p until a minimum value of δ is attained. At $p = 0$, DPA results follow. Figure 2 shows a sample variation of δ with p. This refers to the series F2 and $K = 10$. We notice that a reasonably deep minimum is there. At $p = 0$, we obtain $\delta = 0.1$; the value of δ reduces to 0.0026 at $p = -0.235$. Table 8 shows the performance of both the

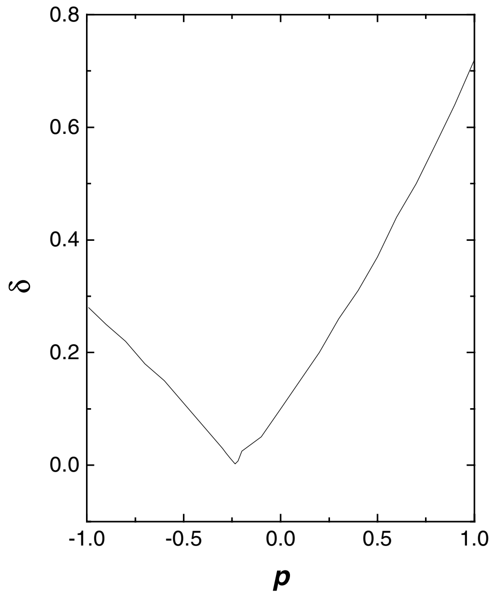

Figure 2. Variation of δ with p (see text) for the series F2 with $K = 10$.

Table 7. Properties of series for self-avoiding walks on a sc lattice ($N = 26$). The odd and even ratios are separately studied. The table shows the last 10 average results.

RM (avg)		SRM (avg)		FRM (avg)	
λ	X	λ	X	λ	X
−1.169 154	0.213 697	−1.166 910	0.213 674	−1.162 597	0.213 620
−1.163 835	0.213 524	−1.161 469	0.213 436	−1.151 402	0.213 339
−1.164 373	0.213 528	−1.174 301	0.213 597	−1.168 438	0.213 556
−1.164 426	0.213 526	−1.169 589	0.213 552	−1.165 961	0.213 531
−1.164 103	0.213 519	−1.165 943	0.213 520	−1.163 103	0.213 506
−1.163 862	0.213 514	−1.164 994	0.213 514	−1.162 875	0.213 504
−1.163 665	0.213 511	−1.164 278	0.213 509	−1.162 631	0.213 502
−1.163 489	0.213 509	−1.163 665	0.213 505	−1.162 334	0.213 501
−1.163 330	0.213 507	−1.163 192	0.213 503	−1.162 094	0.213 499
−1.163 186	0.213 505	−1.162 808	0.213 501	−1.161 886	0.213 498

DPA and the FDPA. Although $T_k^{-1} \equiv T_k(0)^{-1}$ leads finally to a somewhat better value of X than the one provided by the bare sequence, the improvement is not enough. Even the RM yields a superior estimate, as is evident from table 2. Thus, DPA is not recommended in such a situation. The FDPA, on the other hand, performs better than the DPA. The advantage, therefore, is noticeable. The problem of self-avoiding walks will now be briefly considered. Results for the square lattice case are presented in table 9 and those for the sc lattice are shown in table 10. In both situations, we separate the odd and even ratios. In each group, there are 13 terms of a particular sequence, from which we can construct up to [6/6] PA. The tables show how far one can reduce δ by varying p. These separate estimates, on averaging, reveal considerable gains by proceeding through the FDPA. For the square lattice problem, the FDPA performs somewhat inferior to the RM. For the cubic lattice case, however, it works very successfully. Thus, the success of FDPA over the RM depends strongly on the nature of the

Table 8. Improved critical point sequences $\{T_k(p)^{-1}\}$ for the series F2 via the DPA ($p = 0$) and the FDPA ($p = -0.235$) at which δ is minimum. The inverse of the last ratio in the parent sequence is 0.988 61.

	X	
k	T_k^{-1}	$T_k(p)^{-1}$
1	0.947 764	1.001 346
2	0.975 359	0.999 801
3	0.985 748	0.999 626
4	0.990 731	0.999 621
5	0.993 496	0.999 560
6	0.995 188	1.000 060
7	0.996 298	0.999 885
8	0.997 065	0.999 877
9	0.997 586	0.999 872
10	0.997 798	0.999 874

Table 9. Improved critical point sequences $\{T_k(p)^{-1}\}$ for self-avoiding walks on a square lattice via the DPA ($p = 0$) and the FDPA for some p at which δ is minimum. The even and odd ratios are separately studied.

	T_k^{-1}			$T_k(p)^{-1}$		
k	Odd ($\delta = 0.031$)	Even ($\delta = 0.023$)	Avg	Odd ($p = -0.372$) ($\delta = 0.0016$)	Even ($p = -0.229$) ($\delta = 0.0036$)	Avg
1	0.355 932	0.364 784	0.360 358	0.378 739	0.378 570	0.378 654
2	0.378 291	0.371 315	0.374 803	0.378 450	0.377 036	0.377 743
3	0.372 601	0.375 839	0.374 220	0.379 347	0.377 729	0.378 538
4	0.380 346	0.375 599	0.377 973	0.379 281	0.377 616	0.378 449
5	0.376 020	0.376 002	0.376 011	0.379 282	0.378 146	0.378 714
6	0.376 683	0.377 342	0.377 013	0.379 324	0.378 526	0.378 925

Table 10. Critical point sequences $\{T_k(p)^{-1}\}$ for self-avoiding walks on a sc lattice via the DPA ($p = 0$) and the FDPA for some p at which δ is minimum. The even and odd ratios are separately studied.

	T_k^{-1}			$T_k(p)^{-1}$		
k	Odd ($\delta = 0.0104$)	Even ($\delta = 0.0053$)	Avg	Odd ($p = -0.1914$) ($\delta = 0.0008$)	Even ($p = -0.1326$) ($\delta = 0.0003$)	Avg
1	0.206 287	0.209 813	0.208 050	0.213 317	0.213 417	0.213 367
2	0.210 663	0.214 118	0.212 390	0.213 748	0.213 301	0.213 525
3	0.212 028	0.212 235	0.212 131	0.213 750	0.213 237	0.213 493
4	0.212 912	0.212 769	0.212 840	0.213 725	0.213 441	0.213 583
5	0.212 758	0.213 023	0.212 891	0.213 557	0.213 412	0.213 484
6	0.213 005	0.213 008	0.213 007	0.213 571	0.213 412	0.213 491

problem. Nevertheless, it is undoubtedly true that the FDPA works significantly better than the DPA under all circumstances. We can extract roughly two extra correct digits through this scheme. Indeed, at worst, the FDPA would perform similar to the DPA where δ is minimum at $p = 0$. This is a rare possibility.

4. Conclusion

In summary, we have found here a way of modifying certain schemes for obtaining critical indices from power series expansions through the implementation of fractional calculus. Two variants are proposed. We call one the FRM, that goes beyond the RM, and it works well. In many situations, its performance is comparable with another popular prevalent scheme, the SRM. We have established here their kinship too. Our study reveals that there may exist situations where the SRM may perform worse than the parent RM. Table 4 presents a case in point. Genesis of the FRM, in turn, is clear and its workability is always found commendable. The other scheme has its origin in the DPA, and is designated the FDPA. While the performance of the DPA is never found to be comparable with that of any good variant of the RM, we demonstrate here how the FDPA can provide significantly better quality results than the DPA on quite a few occasions. Further exploration of the usefulness of fractional differentiation, especially through (12) and (14), may be worthwhile in the present context.

Acknowledgment

One of us (KB) acknowledges the partial financial assistance of DSA, UGC (India).

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