CHAPTER XV

PROPERTIES OF THE FM: SERIES WITH ZERO CONVERGENCE RADII.

§.49. FM and asymptotic properties of Taylor coefficients of a series with zero convergence radius.

This section starts the analysis of models with power series expansions with zero convergence radius. Our first aim is to apply the formalism developed in §.44 to a simple model with the above features and to determine the conditions under which the FM leads to a convergent sequence.

Let us consider the zero-dimensional field theory model introduced by Eq. (11.14):

$$E(g,\lambda) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-gx^2-\lambda x^4}\, dx \tag{49.1}$$

The coefficients of the λ-power series expansion associated with (49.1) behave asymptotically as shown in Eq. (11.21).

In order to apply the FM, it is first necessary to obtain the dilatation transformation, which in this case happens to be

$$E(g,\lambda) = \frac{1}{\sqrt{\pi}} \lambda^{-1/4} \int_{-\infty}^{+\infty} e^{-g\lambda^{-1/2}x^2-x^4} dx = \lambda^{-1/4}\, E(g\lambda^{-1/2},1) \quad , \tag{49.2}$$

therefore $\beta = -1/4$ and $\alpha = -1/2$. The application of Eqs. (44.7) and (44.3) makes up the starting point to construct the sequence converging towards $E(1,\lambda)$:

G. A. Arteca et al., *Large Order Perturbation Theory and Summation Methods in Quantum Mechanics*

$$E(1,\lambda) = k^{1/2} (1-w)^{1/2} \bar{E}(k,w) ; \bar{E}(k,w) = E(k(1-w),w) \tag{49.3a}$$

$$\lambda = wk^{-2} (1-w)^{-2} \quad . \tag{49.3b}$$

Seznec and Zinn-Justin studied the change of variables (49.3b) to introduce an ODT /1/. Arteca et al /2/ have analysed the connection between both procedures.

According to the function structure (49.1), we obtain from (49.3a) the following result for $\bar{E}(k,w)$

$$\bar{E}(k,w) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-kx^2+w(kx^2-x^4)} \, dx \quad , \tag{49.4}$$

that can be expressed as a w-power series

$$\bar{E}(k,w) = \sum_{n=0}^{\infty} \bar{E}^{(n)} w^n \quad , \tag{49.5a}$$

with coefficients $\bar{E}^{(n)}$ given by

$$\bar{E}^{(n)} = \frac{1}{\sqrt{\pi}n!} \int_{-\infty}^{+\infty} (kx^2-x^4)^n e^{-kx^2} \, dx \quad . \tag{49.5b}$$

As shown in §.43, k must be order-dependent because $E(1,\lambda)$ has zero convergence radius. In order to study such dependence upon the order, we resort to the argument introduced in Ref. /1/. Seznec and Zinn-Justin /1/ determined the parameter k making null the last term in the renormalized series.

Let us apply the saddle-point method (Appendix C) to compute $\bar{E}^{(n)}$. For this purpose, Eq. (49.5b) is rewritten as follows:

$$\bar{\bar{E}}^{(N)} = \frac{1}{\sqrt{\pi}N!} \int_{-\infty}^{\infty} e^{F(x)}\, dx \; ; \; F(x)=-kx^2+N\ln(kx^2-x^4) . \qquad (49.6)$$

The equation determining the F(x) extreme points x* is

$$2kx^{*4} - x^{*2}(2k^2 + 4N) + 2Nk = 0 \quad , \qquad (49.7)$$

which can be rewritten as

$$t^2 - (\delta+2)t + \delta = 0 \quad , \qquad (49.8)$$

where

$$x^{*2} = \alpha t \; ; \; \delta = k/\alpha = k^2/N > 0 \quad . \qquad (49.9)$$

The two roots of Eq. (49.8) are

$$t_{\pm} = \frac{\delta+2}{2} \pm \frac{1}{2}(\delta^2+4)^{1/2} \qquad (49.10)$$

with $0 \leq + < \delta$ and $\delta < t_+ < \infty$.

The replacement of (49.9) in (49.6) yields the F(x) extreme value

$$F(x^*) = F(t) = -Nt + N \ln N + N \ln(t-t^2/\delta) \quad . \qquad (49.11)$$

Taking into account (49.8), the precedent relationship may be written as

$$e^{F(t)} = e^{-Nt} N^N (1- \frac{2t}{\delta})^N \quad . \tag{49.12}$$

The root t_- in (49.10) gives

$$1-\frac{2t_-}{\delta} = t_- - \frac{t_-^2}{\delta} > 0 \text{ since } \delta>t_- \quad , \tag{49.13a}$$

whereupon

$$e^{F(t_-)} = e^{-Nt_-} N^N (1- \frac{2t_-}{\delta})^N > 0 \quad . \tag{49.13b}$$

On the other hand, the second root leads us to

$$1- \frac{2t_+}{\delta} = - \{ \frac{2}{\delta} + (1+ \frac{4}{\delta^2})^{1/2}\} < 0 \quad , \tag{49.14a}$$

after which it follows that $e^{F(t_+)}$ alternates in sign:

$$e^{F(t_+)} = (-1)^N e^{-Nt_+} N^N (\frac{2t_+}{\delta} - 1)^N \tag{49.14b}$$

According to the criterion presented in Ref. /1/, k has to be chosen so that $\bar{E}^{(N)} = 0$. Then, the contributions to the integral coming from the extremes t_+ and t_- must cancel out, i.e.

$$e^{F(t-)} = \gamma e^{F(t_+)} \; ; \; \gamma= e^{im\pi} \quad , \; m = 0, \pm 1 \quad , \tag{49.15}$$

with m = 0 when N is odd and m = $\pm$ 1 when N is even. The substitution of (49.13b) and (49.14b) into (49.15) yields

$$e^{-Nt_-} \left|1- \frac{2t_-}{\delta}\right|^N = \gamma e^{-Nt_+} \left|\frac{2t_\pm}{\delta} -1\right|^N \quad . \tag{49.16}$$

We can select the N-th root of (49.16), considering that

$$\lim_{N\to\infty} \gamma^{1/N} = \lim_{N\to\infty} \{\cos (\frac{m\pi}{N}) + i \sin (\frac{m\pi}{N})\} = 1 \tag{49.17}$$

which leads us to the following equation for large N-values

$$e^{-(t_- - t_+)} = \frac{2t_+ - \delta}{\delta - 2t_-} \tag{49.18}$$

The insertion of Eq. (49.10) into (49.18) determines a trascendental equation in δ:

$$e^{(4+\delta^2)^{1/2}} = \frac{2+(\delta^2+4)^{1/2}}{-2+(\delta^2+4)^{1/2}} \tag{49.19}$$

which has a unique positive real root

$$\delta = 1.3254363337 \quad . \tag{49.20}$$

This allows us to complete the search for the dependence of k upon the order N when N>>1:

$$k^2 \simeq \delta N \quad , \quad \delta \neq \delta(N) \quad . \tag{49.21}$$

Eq. (49.21) is valid for N>1 because it has been determined according to the saddle-point approximation for $\bar{E}$ (k,w).

Next we can compute the asymptotic form of the coefficient $\bar{E}^{(N)}$ by way of Eq. (D.7)

$$\bar{E}^{(N)} \to \frac{1}{N!\sqrt{\pi}} e^{F(t_-)} \left|\frac{2\pi}{-F''(t_-)}\right|^{1/2} , \qquad (49.22)$$

where for the sake of simplicity we have used $t = t_-$.

Eq. (49.6) gives for the second derivative

$$F''(x) = -2k + 2N \frac{k-6x^2}{kx^2-x^4} - 2Nx^2 \left|\frac{k-2x^2}{kx^2-x^4}\right|^2 , \qquad (49.23a)$$

and (49.7) yields

$$F''(x) = -2k + 2N \left|\frac{k-6x^2}{x^2k-x^4}\right| - \frac{4}{N} k^2x^2 . \qquad (49.23b)$$

The replacement of (49.9) into (49.23b) gives the desired result

$$F''(t) = N^{1/2}\{-2\delta^{1/2}-4t_-\delta^{1/2}+2\delta^{1/2}\left|\frac{1-6t_-/\delta}{t_--t_-^2/\delta}\right|\} . \qquad (49.24)$$

Eqs. (49.20) and (49.10) allow us to obtain numerically

$$F''(t_-) = -AN^{1/2} , \quad A = 11.870553667 \qquad (49.25)$$

The substitution of (49.25) and (49.13b) into (49.22) leads us to the following result:

$$\bar{E}^{(N)} \to 2^{1/2} A^{-1/2} N^{-1/4} \frac{N^N}{N!} e^{(1-t_-)^N} (1- \frac{2t_-}{\delta})^N \qquad (49.26)$$

Taking into account the Stirling approximation (Eq. (D.21)), the last equation may be rewritten in a more suitable manner as

$$\bar{E}^{(N)} \to (\pi A)^{-1/2}\, N^{-3/4}\, B^N \quad , \quad B = 0.5154353373 \tag{49.27}$$

The result (49.27) is very important and gives us

$$\lim_{N\to\infty} |\bar{E}^{(N)}| = 0 \tag{49.28a}$$

$$\lim_{N\to\infty} |\bar{E}^{(N)}/\bar{E}^{(N-1)}| = B \tag{49.28b}$$

Although in this case the property (49.28b) does not permit us to compute the convergence radius in w (since we are not dealing with a series but an order-dependent sequence), the analysis performed before shows that (49.5a) converges for $w = 1$. Moreover, Lemma 44.1 assures us that if the sequence converges for $w = 1$, then the same happens for $1/\lambda \to 0$. In other words, the FM sums the λ-power series associated with (49.1) $\forall\ \lambda \geq 0$. Remember that the employed series is asymptotically divergent: $\bar{E}^{(n)} \propto (n-1)!$.

From Eq. (49.27) we can estimate the error arising from the truncation up to the order N. This error is of the order of the last term kept, viz

$$\varepsilon_N = \bar{E}^{(N)} w^N \quad . \tag{49.29}$$

The contribution w^N can be determined from the transformation (49.3b). Noticing that $k\to\infty$ when $N\to\infty$ (Eq. (49.21)), then Eq. (49.3b) yields

$$w \simeq 1 - \frac{1}{k\lambda^{1/2}} + \ldots, \quad k >> 1 \tag{49.30}$$

and thus

$$w^N = e^{N \ln w} \simeq \exp \{N \ln|1- \frac{1}{k\lambda^{1/2}} +....|\} \simeq$$

$$\simeq e^{-N/k\lambda^{1/2}} = e^{-(N/\delta\lambda)^{1/2}} \qquad (49.31)$$

Then, the complete formula for the error is

$$\varepsilon_N = (\pi A)^{-1/2} N^{-3/4} B^N e^{-(N/\delta\lambda)^{1/2}} \quad . \qquad (49.32)$$

In line with the discussion presented in §.44, the largest error corresponds to $1/\lambda \to 0$, that is precisely the condition under which we have tested the convergence.

Up to here we have followed Seznec and Zinn-Justin's criterion and the Saddle-point approximation /1/. Considering the discussion of §.44, the k (=k*) value for the FM must be chosen according to the Sensitivity Rules. Thus, it is important to verify whether the conclusions derived here are also obtained from the Sensitivity Rules for IP and SP sequences. The answer is affirmative, as will be shown in the next paragraph. Some consequences are discussed in Ref. /3/.

It is worth noting that the chosen k value used to prove the convergence of (49.5a) presents a non linear dependence upon the order N (Eq. (47.21)).

Our analysis reveals that such dependence, $k^2 = \delta N$, is essential to get $\varepsilon_N \to 0$ when $N \to \infty$.

Let us now generalize the procedure depicted at the beginning of this section to obtain the expected k-dependence upon the order. We consider a function with a formal divergent asymptotic expansion in λ-power series like (Eq. (11.93)):

$$E(1,\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \ , \ E^{(n)} \to a\, n^b c^n\, (pn+q)! \quad . \qquad (49.33)$$

Assuming a usual scaling law for (49.33), we have

$$E(1,\lambda) = \lambda^{\beta} E(\lambda^{\alpha},1) \qquad (49.34)$$

The FM associates a sequence $S_N(k,w)$ with $E(1,\lambda)$

$$S_N(k,w) = \sum_{n=0}^{N} \bar{E}^{(n)} w^n \qquad (49.35a)$$

where (c.f. Eq. (44.14)):

$$\bar{E}^{(N)} = \sum_{s=0}^{N} (-1)^{N-s} \binom{(s-\beta)/\alpha}{N-s} E^{(s)} k^{(s-\beta)/\alpha} \quad . \qquad (49.35b)$$

Next, we set the last coefficient of (49.35a) equal to zero, and, by using (49.35b), get an approximate behavior for k:

$$k^{N/\alpha} E^{(N)} \simeq \text{constant } k^{(N-1)/\alpha} E^{(N-1)} \qquad (49.36)$$

The substitution of (49.33) into (49.36) allows us to deduce the k dependence upon the order:

$$\rho = k^{-1/\alpha} \simeq \delta N \qquad (49.37)$$

If $\alpha = -1/2$, then it follows Eq. (49.21). Eq. (49.37) shows the sort of k dependence on N to be expected in order to have a convergent sequence $S_N(k,1)$ (and from it SE_N). As stated before such k vs N dependence is determined through a dilatation relationship and the knowledge of the approximate asymptotic behavior of the coefficients $E^{(n)}$.

It seems that the convergence rate of power series by these order-dependent transformations depends on the α and β exponents. In Appendix J we provide an analysis of the conformal mappings between λ and w complex planes, as functions of α and β. As it is shown there, these transformations remove a growing number of singularities in λ from inside the convergence domain when N increases. The way and rate with which these λ-singularities are removed depends on α and β, and fixes the efficiency of the FM as a summation method. We propose in Appendix J an approximate quantitative measure for such an efficiency, as a function of the exponents characterizing the Symanzik scaling law.

§.50. Application of the FM to integrals of interest in field theory and statistical mechanics.

Let us consider again the field theory elementary model (49.1) to study numerically the λ-power series convergence by the FM.

The model defined by

$$E(1,\lambda) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-(x^2+x^4\lambda)} dx = \lambda^{-1/4} E(\lambda^{-1/2},1) \quad , \qquad (50.1)$$

has two associated power series expansions

$$E(1,\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \; ; \; E^{(n)} = (-1)^n \frac{(4n)!}{n!(2n)!2^{4n}}, \lambda \to 0 \quad , \qquad (50.2a)$$

$$E(1,\lambda) = \lambda^{-1/4} \sum_{n=0}^{\infty} e^{(n)} \lambda^{-n/2} \; ; \; e^{(n)} = (-1)^n (2n-\tfrac{3}{4})!/$$

$$2\pi^{1/2} n!) \; ; \; \frac{1}{\lambda} \to 0 \quad . \qquad (50.2b)$$

We choose the expansion (50.2a) and analyse the convergence behavior of the renormalized series when $1/\lambda \to 0$. In line with equations presented in §.44, the FM approches to $E(1,\lambda)$ through the sequence

$$E(1,\lambda) \simeq SE_N = k^{1/2} (1-w)^{1/2} S_N(k,w) \quad , \qquad (50.3a)$$

$$S_N(k,w) = \sum_{n=0}^{N} \bar{E}^{(n)} w^n \quad , \qquad (50.3b)$$

where w is a root of Eq. (44.7), i.e.

$$\lambda k^2 w^2 - w(1+2\lambda k^2) + \lambda k^2 = 0 \quad . \qquad (50.3c)$$

According to the Lemma (44.2) the chosen root is

$$w = \frac{1}{2\lambda k^2}\{1 + 2\lambda k^2 - (1 + 4\lambda k^2)^{1/2}\} \quad . \qquad (50.3d)$$

Coefficients $\bar{E}^{(n)}$ arise from Eq. (44.14), and for the model (50.1) they are

$$\bar{E}^{(n)} = \sum_{s=0}^{n} (-1)^{n-s} \binom{-(4s+1)/2}{n-s} E^{(s)} k^{-(4s+1)/2} \quad . \qquad (50.3e)$$

The k-value must be determined according to the Sensitivity Rules by studying the critical points of the sequence $S_N(k,1)$

$$S_N(k,1) = \sum_{n=0}^{N} \bar{E}^{(n)} \quad . \qquad (50.4)$$

When analysing the convergence of SE_N toward $E(1,\lambda)$, the most unfavourable condition corresponds to the case $1/\lambda \to 0$. Thus, one can expect that $S_N(k,1)$ converges to $\lambda^{1/4}\, E(1,\lambda)$, i.e.

$$S_N(k,1) \to e^{(0)} = \Gamma(1/4)/2\pi^{1/2} = 1.022765672... \qquad (50.5)$$

The computational procedure is quite simple. The first and second derivatives of (50.4) are obtained at once from (50.3e):

$$\frac{d}{dk} S_N(k,1) = -\frac{1}{2} \sum_{n=0}^{N} \sum_{s=0}^{n} (-1)^{n-s} (4s+1) \binom{-(4s+1)/2}{n-s} E^{(s)} k^{-(4s+3)/2} ,$$

(50.6a)

$$\frac{d^2}{dk^2} S_N(k,1) = \frac{1}{4} \sum_{n=0}^{N} \sum_{s=0}^{n} (-1)^{n-s} (4s+1)(4s+3) \binom{-(4s+1)/2}{n-s} E^{(s)} k^{-(4s+5)/2} .$$

(50.6b)

After determining the zeros of (50.6a) and (50.6b) for N = 1,2,... the Sensitivity Rules yield the optimum parameters k_N^S and k_N^I which allow us to study the convergence (50.5). Finally,Eqs. (50.3a), (50.3b) and (50.3d) give the approximation to the function $E(1,\lambda)$.

Before discussing the numerical results, it is suitable to make some general comments on the computational procedure:

i) A very simple computer program is needed to determine the roots of Eqs. (50.6a) and (50.6b) for N = 1,2,...

ii) Intrinsic errors in the computational scheme can be further reduced by determining k_N up to 15 significant figures and using double precision.

iii) A binary bisection algorithm is employed to compute the zeros of (50.6a) and (50.6b), since although it is slower than other approximation procedures, it does not present major convergence problems.

iv) The greatest limitation regarding the accuracy of the results for $S_N(k,1)$ lies in the accuracy of the coefficients $E^{(n)}$. Our computational experience comfirms up to a good degree a rule pointed out by Le Guillou and Zin-Justin /4/ when studying the Zeeman effect in hydrogen. This rule may be stated as follows: to approach in an efficient way the function under consideration by means of a sum method and 2N terms of the RSPT, then the RS coefficients must be known up to N significant figures.

For the model (50.1), coefficients $E^{(n)}$ are known with the desired accuracy for any n, so that round off and truncation errors of the particular computer machine must be considered. It is more convenient to compute them in a recursive manner:

$$E^{(n)} = - \frac{(4n-1)(4n-3)}{4n} E^{(n-1)} \quad , \; n > 1 \quad . \qquad (50.7)$$

Eq. (50.7) allows us to compute up to $E^{(24)} \simeq 1,6 \times 10^{37}$ without making any further modification. The maximum figure N = 24 is large enough for our convergence analysis

Table 15.1: Convergent renormalized sequences obtained by means of the FM for the integral (50.1).

N	k_N^S a)	$S_N(k_N^S,1)$ a)	k_N^S b)	$S_N(k_N^S,1)$ b)
1	1.5811383301	0.954325		
2			2.2750692367	0.988061
3	2.2686203055	1.01093		
4			2.7262835278	1.01714
5	2.7921625419	1.02036		
6			3.1595269728	1.02163
7	3.2320935106	1.02224		
8			3.5477633258	1.02252
9	3.6189740554	1.02265		
10			3.9000505775	1.02271
11	3.9683323435	1.02274		
12			4.2241693568	1.02275

13	4.2893393194	1.02275898		
14			4.5257119252	1.02276249
15	4.5879464926	1.02276405		
16			4.8087160792	1.02276490
17	4.868275699	1.02276528		
18			5.0761745862	1.02276548
19	5.1333196163	1.02276557		
20			5.3303680520	1.02276563
21	5.3853608114	1.02276565		
22			5.5729670487	1.022765661
23	5.6259528357	1.022765666		
24			5.8062772752	1.022765669

a) Sequence A.

b) Sequence B.

Table 15.1 (cont.)

N	k_N^I c)	$S_N(k_N^I,1)$ c)
1	2.41522945772	0.882458
2	3.34026841135	0.911606
3	4.45010636123	0.915744
4	5.57824977631	0.917569
5	6.71611510403	0.918499
6	7.85917109226	0.919037
7	9.00532549791	0.919377
8	10.1534807862	0.919605
9	11.3030048228	0.919766
10	12.4535072544	0.919884
11	13.6047337191	0.919972
12	14.7565112320	0.920041
13	15.9087179817	0.920095
14	17.0612656726	0.920138
15	18.2140887189	0.920173
16	19.3671373726	0.929292
17	20.5203732075	0.920227
18	21.6737660678	0.920247
19	22.8272919532	0.920265
20	23.9809315232	0.920280
21	25.1346690179	0.920293
22	26.2884914640	0.920304
23	27.4423880853	0.920314
24	28.5963498558	0.920323

c) Sequence C.

Table (15.1) shows results for k_N^* and $S_N(k_N^*,1)$, $1 \leq N \leq 24$. It is to be noted that whenever N is even, $S_N(k,1)$ only presents two IP, while for the case N odd there are one IP and one SP. Thus, we have two convergent sequences through IP and one from the SP, which can be arranged according to their dependence upon the order N.

The dependence of k_N^* on N for the several sequences is numerically fitted by means of a regression analysis /5/. In the following we call A,B,C to the sequence through the SP and the two sequences from the IP, respectively,

From the last six values for the A sequence, we find the dependence (N odd):

$$(k_N^S)^2 = (1.169 \pm 0.001) + (1.3253 \pm 0.0003)\ N \qquad (50.8a)$$

$$r = 0.9999999952 \quad , \qquad (50.8b)$$

where r is the correlation coefficient /5/. It must be pointed out that in order to obtain the accidental errors (50.8a), we have employed a 99% confidence interval.

The result obtained from the last six values of the sequence B (even) is

$$(k_N^I)^2 = (1.958 \pm 0.008) + (1.323 \pm 0.002)\ N \qquad (50.9a)$$

$$r = 0.99999971 \quad . \qquad (50.9b)$$

Finally, the sequence C (for any N) gives for the last 12 values a different dependence.

$$k_N^I = (0.912 \pm 0.003) + (1.1534 \pm 0.0007)\ N \qquad (50.10a)$$

$$r = 0.999999934 \quad . \tag{50.10b}$$

Results (50.8) - (50.10) are very suggestive and they permit us to extract important conclusions, which are displayed in what follows:

i) The method permits one to obtain, from a Taylor expansion with zero convergence radius, order-dependent convergent sequences depending on the order. The structure of such dependence upon the order is determined in a natural way by the Sensitivity Rules for the $S_N(k,1)$ critical points.

ii) Among the three sequences, two of them predict a perfect linear correlation between k^2 and N, which is in agreement with the expected behavior for this model according to Eq. (49.37). As well, as discussed in §.47, there appears a sequence with linear correlation between k and N.

iii) The numerical fitting made for the linear correlations $k^2 = \delta N$ in the A and B sequences allows us to obtain as the most accurate result

$$\delta = 1.3253 \pm 0.0003 \tag{50.11}$$

which is in excellent agreement with Eq.(49.20). Let us recall this last equation was derived from a completely different procedure: to make null the last coefficient of the renormalized series /1/.

iv) A and B sequences converge uniformly from below toward the exact result (50.5). Table 15.1 gives the following results

$$S_{23}(k^S_{23},1) = 1.022765666 \text{ , sequence A} \tag{50.12a}$$

$$S_{24}(k^I_{24},1) = 1.022765669 \text{ , sequence B} \tag{50.12b}$$

For N = 24 we find an error of about 3×10^{-9} with respect to the exact result. For the sake of comparison, Eq. (49.32) yields the following error when $1/\lambda \to 0$ (predicted from the saddle point argument):

$$\varepsilon_{24} = 1,9 \times 10^{-9} \quad . \tag{50.13}$$

The agreement is noteworthy, revealing that the FM allows one to obtain the expected convergence rate through its critical point sequences. Likewise, we may note that our predictions about the Sensitivity condition (plateau) for $S_N(k,1)$ as a k-function is fulfiled quite well: the second derivatives decrease permanently following a sequence of SP's, and the same happens for the first derivative via a sequence of IP's.

v) Sequence C (which has a k vs N linear dependence) converges to an incorrect result from below the exact one. We can estimate in an approximate fashion that

$$S_N(k_N^I,1) \simeq 0.9203 \pm 0.0001, \; N>>1 \tag{50.14}$$

Though the model (50.1) has been studied by several authors with order-dependent transformations, the three sequences (50.12a), (50.12b) and (50.14) are completely original (see Ref. /3/).

vi) Results (50.12) assures us that for $\lambda<\infty$ we have an approximation to the exact result $E(1,\lambda)$ with 9 decimal places at least. In order to perform this calculation, we show in Table 15.2 the coefficients $\bar{E}^{(n)}$ obtained by means of k_{24}^S of the sequence B.

Table 15.2: Coefficients $\bar{E}^{(n)}$ of the renormalized series for the model (50.1) up to the 24th-order.

n	$\bar{E}^{(n)}$ a)		n	$\bar{E}^{(n)}$	
0	0.415002883507	(0)	13	0.40476199735	(-3)
1	0.198268994508	(0)	14	0.18336771682	(-3)
2	0.133743080530	(0)	15	0.7953303026	(-4)
3	0.943947765661	(-1)	16	0.3312447890	(-4)
4	0.659163380150	(-1)	17	0.132364863	(-4)
5	0.446492425652	(-1)	18	0.59834208	(-5)
6	0.290791541167	(-1)	19	0.18782714	(-5)
7	0.181312788840	(-1)	20	0.6683934	(-6)
8	0.108006956255	(-1)	21	0.229294	(-6)
9	0.61416078404	(-2)	22	0.7595	(-7)
10	0.33332446288	(-2)	23	0.2416	(-7)
11	0.17272408240	(-2)	24	0.784	(-8)
12	0.85509054517	(-3)			

a) Figures must be multiplied by a power of ten given between parenthesis. Results were rounded off according to the significant figures given for k_{24}^{I}.

The FM permits a straightforward calculation of $E(1,\lambda)$, since coefficients $\bar{E}^{(n)}$ are determined just once. Table (15.3) displays the results for SE_{24} as an approximation to $E(1,\lambda)$ in a wide range of λ-values. This computation was accomplished via Eqs.(50.3a), (50.3b) and (50.3d), and the approximate results are compared with the exact ones (determined with the Romberg integration method).

Table 15.3 : Results obtained for the function (50.1) in a wide range of λ-values.

λ	$E(1,\lambda)$ exact [a)]	SE_{24} [b)]
10^{-4}	0.9999250328	0.9999250328
10^{-3}	0.9992532545	0.9992532545
10^{-2}	0.9928039079	0.9928039080
10^{-1}	0.9445918017	0.9445918016
1	0.7720521778	0.7720521778
10	0.5201607637	0.5201607634
10^{2}	0.3128864550	0.3128864541
10^{3}	0.1799548854	0.1799548843

a) Numerically computed by the Romberg integration method.

b) Calculated with the coefficients from Table 15.2.

A careful look at Table 15.3 allows one to verify that all previous predictions are fulfiled. Results obtained through the FM are better, regarding accuracy and convergence rate, than those derived from the use of the Padé and Borel-Padé methods /6/. Taking into account that (50.1) describes a classical partition function for an anharmonic quartic oscillator /7/, we can conclude the FM permits one to have up to a considerable accuracy degree such a function for any temperature (proportional to λ).

A closely related problem with (50.1) is that one determined by the anharmonic mean quadratic displacement function

$$\langle x^2 \rangle = \int_0^\infty x^2 \, e^{-\beta' V(x)} dx \Big/ \int_0^\infty e^{-\beta' V(x)} dx \quad , \qquad (50.15)$$

where V(x) is quartic anharmonic potential

$$V(x) = v_2x^2 + v_4x^4 \qquad , \qquad (50.16a)$$

and

$$\beta' = (k'T)^{-1} \qquad , \qquad (50.16b)$$

with k' the Boltzmann constant and T the absolute temperature. Function (50.15) has been thoroughly studied because it is useful to interpret several experimental data such as the dynamical answer of ferroelectric materials, of order-disorder and displaceable type /8/, as well as the dependence upon the temperature of the isocoric dielectric polarizability of some liquids /9,10/. The relationship between the function (50.15) and the polarizability of any material medium is discussed in Appendix K.

Owing to the deep interest about expression (50.15) there have been several alternative proposals to derive simple and accurate formulas to compute it as a function of the temperature /10,11/. The FM is particularly suitable to obtain analytical expressions for this specific function, due to its similitude with (50.1).

Function (50.15) has been recently studied /12,13/ by means of the formalism developed in §.42.

In order to apply the FM it is convenient to rewrite (50.15) as follows (see Appendix K):

$$E(1,\lambda) = 2\beta' v_2 \langle x^2 \rangle = \int_0^\infty x^2 e^{-(x^2+\lambda x^4)} dx \Big/ \int_0^\infty e^{-(x^2+\lambda x^4)}\, dx \qquad , \qquad (50.17a)$$

$$\lambda = v_4/(\beta' v_2^2) \qquad . \qquad (50.17b)$$

Notice that the study of the behavior $1/\lambda \to 0$ in $E(1,\lambda)$ corresponds to the function (50.15) at the limit $T \to \infty$.

Function (50.17) obeys a scaling law

$$E(1,\lambda) = \lambda^{-1/2} E(\lambda^{-1/2},1) \qquad (50.18)$$

which follows at once from the change of variables $y^4 = \lambda x^4$. Eq.(50.13) provides the exponents $\alpha = \beta = -1/2$ (see Appendix J). In order to use the FM, we have at our disposal the expansions (50.17) in λ and $\lambda^{-1/2}$ power series. Keeping only up the first coefficients /11-14/ we are led to

$$E(1,\lambda) = 1-3\lambda + 24\lambda^2 - 297\lambda^3 + 4896\lambda^4 - 100273\lambda^5 + \ldots =$$

$$= \sum_{n=0}^{\infty} E^{(n)} \lambda^n \quad , \qquad (50.19a)$$

$$\lambda^{1/2}E(1,\lambda) = 0.6759782399-0.2715267096\ \lambda^{-1/2} + 0.07722148863\ \lambda^{-1} -$$

$$- 0.0155666445\ \lambda^{-3/2} + 0.00173008354\ \lambda^{-2} - \ldots = \sum_{n=0}^{\infty} e^{(n)}\ \lambda^{-n/2} .$$

(50.19b)

The expansion (50.19a) has a zero convergence radius, although appropriately rewritten as a continuum fraction it is convergent /10/ (see also Appendix K). However, the employment of the continuum fraction is not convenient since it converges very slowly for $\lambda \geq 1$. For example, to obtain a reasonable result for $\lambda = 10$, it is necessary to use around 200 terms in the continuum fraction /10/.

We have only introduced the first terms of the expansions (50.19) so as to make a direct comparison with the results reported by Booth

/11/, which up to now are the most accurate analytical expressions in the current literature. Booth resorted to the following expression to approximate (50.17):

$$E(1,\lambda) \simeq \sum_{i=0}^{n} a_i(\lambda+c_i^2)^{-1/2} \quad . \qquad (50.20)$$

The 2n parameters a_i and c_i are adjusted in such a way that (50.20) fulfils the following relationships:

$$\frac{1}{i!}\left(\frac{d^iE}{d\lambda^i}\right)(\lambda = 0) = E^{(i)} \quad , \quad i = 0,1,2,\ldots,2n-1 \; , \qquad (50.21a)$$

$$\lim_{\lambda\to\infty} \lambda^{1/2} E = e^{(0)} \quad . \qquad (50.21b)$$

It must be pointed out that (50.20) allows one to use the combined information arising from both λ-series expansions (Eqs. (50.19)). However, (50.20) has a serious drawback leading to a $\lambda^{-1/2}$ power series expansion when $\lambda\to\infty$, as required by the function $E(1,\lambda)$. We know that the FM permits one in a natural and direct way to include both expansions.

The use of Eqs. (44.8) and (44.13), together with the coefficients α and β, lead to the approximation given by the FM for the function (50.17):

$$SE_N = k(1-w)\; S_N(k,w) \qquad (50.22a)$$

$$S_N(k,w) = \sum_{n=0}^{N} \bar{E}^{(n)}\; w^n \qquad (50.22b)$$

The variable w is given by (50.3d) since the models (50.1) and (50.17) are characterized by $\alpha = -1/2$, Eq.(44.17) furnishes the coefficients $\bar{E}^{(n)}$:

$$\bar{E}^{(n)} = \sum_{j=0}^{n} \binom{j+n}{2j} E^{(j)} k^{-(2j+1)} \qquad (50.22c)$$

In order to perform a full comparison with formula (50.20) we incorporate $e^{(0)}$ in our computations before determining k* in agreement with the Sensitivity Rules. The introduction of the coefficient $e^{(0)}$ may be made in an analogous fashion as done in Eq. (46.17), resorting to the procedure developed at the end of section §.42. The necessary steps to be followed are:

i) From the five coefficients in (50.19a) we determine $\bar{E}^{(0)}$, $\bar{E}^{(1)}, \ldots, \bar{E}^{(5)}$.

ii) $e^{(0)}$ is added by way of $\bar{E}^{(6)}$, using Eq. (46.16), which in this present case is

$$\bar{E}^{(6)} = e^{(0)} - \sum_{n=0}^{5} \bar{E}^{(n)} \quad . \qquad (50.23)$$

The approach to (50.17) will be denoted as SE_6', where the prime symbol is affixed to denote that $\bar{E}^{(6)}$ in (50.22b) is given by (50.23). The k-optimum value (k*) is chosen as an IP or SP of the sequence SE_6' This particular example presents a stationary point at k* = 3.2628, independently of λ. These values are used to compute SE_6' (k*,w) and the results are compared in Table 15.4 with respect the exact ones (determined with the Romberg's integration method) and those reported by Booth /11/ (obtained with the same number of coefficients). Evidently, our results are far superior in quality, within the whole range of λ-values.

Table 15.4: Compared results for the classic statistical average value of the quadratic shift in the quartic anharmonic oscillator, Eq. (50.17), for a wide range of λ-values.

λ	$E(1,\lambda)$ exact [a)]	$E(1,\lambda)$ [b)]	SE'_6 [c)]
10^{-4}	0.9997002	0.99970	0.9997002
10^{-3}	0.997024	0.99702	0.997024
10^{-2}	0.972144	0.97214	0.972144
10^{-1}	0.817561	0.81858	0.817558
1	0.467919	0.48921	0.467901
10	0.188902	0.20276	0.188896
10^2	0.064958	0.06721	0.064957
10^3	0.0211072	0.02136	0.0211071

a) Results determined by way of a numerical integration via the Romberg method.

b) Eq. (50.20) with n = 3 (Ref./11/).

c) Results determined with the FM (Eq.(50.24)), k*=3.2628.

Summing up, we have shown that the FM provides an accurate approximation to the classical statistical average value of the means square displacement in a quartic anharmonic oscillator for arbitrary temperatures. Results were obtained from a T-power series expansion which has a zero convergence radius.

Since sometimes it is necessary to have accurate analytical expressions for $E(1,\lambda)$, we write here the formula provided by the FM (used to make the computations presented in Table 15.4):

$$E(1,\lambda) \simeq SE_6' = 3.2628\ (1-w)\ \{0.3064852274 + 0.2201178179w +$$

$$+ 0.01122851323\ w^2 + 0.0373476866\ w^3 + 0.0050596001\ w^4 -$$

$$- 0.0032274428\ w^5 - 0.0020897815\ w^6\ \} \quad , \qquad (50.24)$$

where w is given by (50.3d) with $k = k^* = 3.2628$. The comparison of (50.24) with the original series (50.19a) plainly reveals the advantages in the use of the FM because the function is represented as a power series of a parameter $|w|<1$ with coefficients decreasing in absolute value when the order increases.

§.51. Convergence conditions for the FM: Discussion of integrals with factorial divergence.

We have discussed in preceding sections some functions of interest in Physical Chemistry, which have associated power series expansions with zero convergence radius. These problems can be studied in an approximate fashion up to a good accuracy degree via the FM from the knowledge of a scaling law. Furthermore, the functions analysed in §.§. 49 and 50 fulfil an additional condition, viz. they present power series expansions for both regimes of the λ parameter.

The purpose of this section is to study the convergence properties when one employes the FM to sum the power series about $\lambda = 0$, for those functions that cannot be expanded in power series about $1/\lambda = 0$.

Once again, simple functions are chosen so as all the computations can be performed in an analytical manner. Nevertheless, the conclusions to be derived are also valid when more involved problems are considered.

Let us consider a function $E(Z,\lambda)$, for $|\arg(\lambda)|<\pi$ and having an associated asymptotic divergent expansion in λ-power series

$$E(Z,\lambda) = \sum_{n=0}^{\infty} E^{(n)}\lambda^n, \quad E^{(n)} = E^{(n)}(Z) \quad , \qquad (51.1)$$

with the property

$$\lim_{|\lambda|\to\infty} E(Z,\lambda) = 0 \quad . \qquad (51.2)$$

For the time being, we shall not discuss the role of the Z parameter which is chosen equal to one.

Function $E(1,\lambda)$ may be represented as a Cauchy integral using the integration path as shown in Fig. 4.2.:

$$E(1,\lambda) = \frac{1}{2\pi i} \int_C \frac{E(1,x)}{x-\lambda} \, dx \quad , \qquad (51.3)$$

where C avoids the singularity at $|\arg(k)| = \pi$. Using the same notation as in Fig. 4.2., and the property (51.2), Eq. (51.3) changes into

$$E(1,\lambda) = \frac{1}{2\pi i} \lim_{\substack{r\to 0\\ R\to\infty}} \oint_C \frac{E(1,x)}{x-\lambda} \, dx = \int_{-\infty}^{0} \frac{D(x)}{x-\lambda} \, dx \quad , \qquad (51.4a)$$

where

$$D(x) = \frac{1}{2\pi i} \lim_{\varepsilon\to 0} \{E(1,x+i\varepsilon) - E(1,x-i\varepsilon)\} = \frac{\mathrm{Im}E(1,x)}{\pi} \quad . \qquad (51.4b)$$

Eq. (51.4b) can be rewritten in a more suitable way so as to obtain an integral representation for $E(1,\lambda)$:

$$E(1,\lambda) = -\int_0^{\infty} \frac{D(-x)}{x+\lambda} \, dx = \int_0^{\infty} \frac{G(t)}{1+\lambda t} \, dt \quad , \qquad (51.5a)$$

with

$$t = x^{-1} \ , \ G(t) = - D(-t^{-1})t^{-1} \quad . \tag{51.5b}$$

Eq. (51.5a) is an integral representation of $E(1,\lambda)$, and may be employed to generate the λ-power series expansion. The expansion of the denominator of (51.5a) as a λ-power series and the identification term by term with Eq. (51.1) yields:

$$E^{(n)} = (-1)^n \int_0^\infty t^n \, G(t) \, dt \quad . \tag{51.6}$$

Functions $E(1,\lambda)$, whose expansions (51.1) diverge as

$$E^{(n)} = (-1)^n \, \Gamma \, (An+B) = (-1)^n \, (An+B-1)! =$$

$$= (-1)^n \int_0^\infty t^{An+B-1} \, e^{-t} \, dt \quad , \tag{51.7}$$

are especially interesting and will be considered in what follows.

The equality between (51.7) and (51.6) gives the $E(1,\lambda)$ representation, whose power series expansion has the property (51.7):

$$E(1,\lambda) = \int_0^\infty \frac{t^{(A-1)n+B-1}}{1+\lambda t} \, e^{-t} \, dt \quad . \tag{51.8}$$

Let us consider a series whose coefficients are

$$E^{(n)} = (-1)^n \, n! \quad , \quad A = B = 1 \quad . \tag{51.9}$$

This function can be generated as follows:

$$E(Z,\lambda) = \int_0^{\infty} \frac{e^{-t}}{Z+\lambda t}\, dt \quad . \tag{51.10}$$

The function $E(Z,\lambda)$ evidently satisfies the dilatation relationship

$$E(Z,\lambda) = \lambda^{-1} E(Z\lambda^{-1},1) = Z^{-1} E(1,\lambda Z-1) \quad . \tag{51.11}$$

The integral (51.10) is not expandable in λ^{-1}-power series. Besides, $\lambda E(1,\lambda)$ does not remain finite when $1/\lambda = 0$, so that such behavior cannot be described by the FM of §.44. Let us analyse the way (51.10) diverges when $1/\lambda \to 0$. The change of variables $y = (1+\lambda t)/\lambda$ in (51.10) yields:

$$E(1,\lambda) = \frac{e^{1/\lambda}}{\lambda} \int_{1/\lambda}^{\infty} \frac{e^{-y}}{y}\, dy \quad . \tag{51.12}$$

It is convenient to rewrite Eq. (51.12). We start from the following relationship

$$\int_{1/\lambda}^{\infty} \frac{e^{-y}}{y}\, dy = \int_1^{\infty} \frac{e^{-y}}{y}\, dy + \int_1^{1/\lambda} \frac{1-e^{-y}}{y}\, dx - \int_1^{1/\lambda} \frac{dy}{y} \; ; \tag{51.13a}$$

The subsequent power series expansion leads to

$$\int_{1/\lambda}^{\infty} \frac{e^{-y}}{y}\, dy = - \ln\left(\frac{1}{y}\right) - C_1 - C_2 + \sum_{n=0}^{\infty} (-1)^n \frac{(1/\lambda)^{n+1}}{(n+1)(n+1)!} \tag{51.13b}$$

where C_1 and C_2 are constants given by

$$C_1 = \int_1^{\infty} e^{-y}\, y^{-1}\, dy \; ; \; C_2 = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)\,(n+1)!} \qquad (51.13c)$$

Replacing (51.13b) into (51.12a), we get the $E(1,\lambda)$ asymptotic behavior

$$E(1,\lambda) \to e^{1/\lambda}\, \frac{\ln\lambda}{\lambda} + \frac{e^{1/\lambda}}{\lambda} \left\{ -(C_1+C_2) + \sum_{n=0}^{\infty} (-1)^n \frac{\lambda^{-(n+1)}}{(n+1)\,(n+1)} \right\} \quad .$$

(51.14)

Due to the presence of the factor $\frac{\ln\lambda}{\lambda}$ in (51.14), the FM cannot be applied to study the convergence behavior of the sequence SE_N when $1/\lambda \to 0$.

In order to apply the FM it is necessary that $E(1,\lambda)$ remains finite for $1/\lambda = 0$. For that purpose we consider an expansion with coefficients

$$E^{(n)} = (-1)^n\, (n+1)! \quad , \quad A = 1, \; B = 2 \qquad (51.15)$$

arising from the function (Z=1)

$$E(Z,\lambda) = \int_0^{\infty} \frac{te^{-t}}{Z+\lambda t}\, dt \quad . \qquad (51.16)$$

Function (51.16) fulfils the same scaling law (51.11) as (51.10), but here

$$\lim_{\lambda\to\infty} \lambda E(1,\lambda) = 1 \qquad (51.17)$$

Let us analyse how the FM allows one to approximate the limit (51.17) using the λ-power series. We start analysing the renormalized series, so we write the following expression from Eq. (51.16)

$$\bar{E}(k,w) = E(k(1-w),w) = \int_0^\infty \frac{xe^{-x}}{k-kw+wx}\,dx = \frac{1}{k}\int_0^\infty \frac{xe^{-x}}{1+\frac{w}{k}(x-k)}\,dx \;, \qquad (51.18a)$$

and its associated power series expansion

$$\bar{E}(k,w) = \sum_{n=0}^{\infty} \bar{E}^{(n)}\, w^n \;;\; \bar{E}^{(n)} = \frac{1}{k}\int_0^\infty x(1-\frac{x}{k})^n\, e^{-x}\, dx \quad , \qquad (51.18b)$$

with

$$w = \lambda k/(1+\lambda k) \quad . \qquad (51.18c)$$

Let us determine the conditions under which $\lim_{N\to\infty} \bar{E}^{(N)} = 0$. To this end, we write the N-th coefficient as follows:

$$\bar{E}^{(N)} = I_1 + I_2 \qquad (51.19a)$$

$$I_1 = \frac{1}{k}\int_0^k x(1-\frac{x}{k})^N\, e^{-x}\, dx \;;\; I_2 = \frac{1}{k}\int_k^\infty x(1-\frac{x}{k})^N\, e^{-x}\, dx \quad . \qquad (51.19b)$$

Considering that $(1-\gamma)^N < e^{-N\gamma}\ \forall\ \gamma < 1$, we can find a bound for the integral $I_1 (x<)$:

$$0 < I_1 < \frac{1}{k}\int_0^k xe^{-(1+N/k)x}\, dx < \frac{1}{k}\int_0^\infty xe^{-(1+N/k)x}\, dx = \frac{k}{(N+k)^2} \qquad (51.20a)$$

Regarding the integral I_2 it is convenient to change the integration interval to $(0,\infty)$ making $y = x - k$:

$$I_2 = \frac{e^{-k}}{k} \int_0^\infty (-1)^N (\frac{y}{k})^N \ (y+k) \ e^{-y} \ dy =$$

$$= \frac{e^{-k}}{k} \{ (- \frac{1}{k})^N \int_0^\infty y^{N+1} \ e^{-y} \ dy - (- \frac{1}{k})^{N-1} \int_0^\infty y^N e^{-y} \ dy \} =$$

$$= (-1)^N \ k^{-(N+1)} \ (N+1)! \ e^{-k} \ \{1 + \frac{k}{N+1} \} \tag{51.20b}$$

so that it follows the bound

$$|I_2| < \frac{(N+1)!}{k^{N+1}} \{1 + \frac{k}{N+1}\} \quad . \tag{51.20c}$$

Finally we have

$$0<|\bar{E}^{(N)}| = |I_1+I_2| < |I_1| + |I_2| < \frac{(N+1)!}{k^{N+1}} (1 + \frac{k}{N+1}) +$$

$$+ \frac{k}{(N+k)^2} \quad . \tag{51.21}$$

Evidently, Eq. (51,21) shows that $\bar{E}^{(N)}$ remains finite when $N\to\infty$ if k depends properly upon the order N. Let us introduce a dependence on the order like

$$k = \delta N^r \ , \ r > 0 \tag{51.22}$$

and look for the r-values that make $\bar{E}^{(N)}$ zero when $N\to\infty$. The substitution of (51.22) in (51.20b), and the application of the Stirling approximation (Appendix D) yields

$$|I_2| \to N^{N(1-r)}\ \delta^{-(N+1)}\ \{1+\delta N^{r-1}\} e^{-(N+1+\delta N^r)}\ ;\ N>>1\ . \quad (51.23)$$

which immediately gives

$$\lim_{N\to\infty} |I_2| = 0 \text{ when } r \geq 1 \quad , \quad (51.24a)$$

$$\lim_{N\to\infty} |I_2| = \infty \text{ when } 0<r<1 \quad . \quad (51.24b)$$

On the other hand, the replacement of (51.22) into (51.20a) yields

$$|I_1| < \frac{\delta N^r}{(N+\delta N^r)^2} \quad , \quad (51.25)$$

and thus

$$\lim_{N\to\infty} |I_1| = 0\ ;\ r>0 \quad . \quad (51.26)$$

The use of (51.24), and (51.26) in (51.21), allows us to find out the desired relation

$$\lim_{N\to\infty} |\bar{E}^{(N)}| = 0 \text{ when } r\geq 1 \quad (51.27a)$$

$$\lim_{N\to\infty} |\bar{E}^{(N)}| = \infty \text{ when } 0<r<1 \quad . \quad (51.27b)$$

Eq. (51.27b) assures us that (51.18b) does not converge for $1/\lambda\to 0$ $(w\to 1)$ if $r<1$.

In order to study the convergence when $r \geq 1$, we resort to the renormalized sequence $S_N(k,w)$ truncating (51.13b), i.e.

$$S_N(k,w) = \sum_{n=0}^{N} \bar{E}^{(n)} w^n = \frac{1}{k} \int_0^\infty xe^{-x} \sum_{n=0}^{N} w^n (1-\tfrac{x}{k})^n \, dx \tag{51.28}$$

Making use of the partial sum of the geometrical series (Eq.(47.3)), Eq. (51.28) may be transformed into

$$S_N(k,w) = \frac{1}{k} \int_0^\infty x \, \frac{1-(1-x/k)^{N+1} \, w^{N+1}}{1-(1-x/k)w} \, e^{-x} \, dx \quad . \tag{51.29}$$

The renormalized sequence (51.29) should converge to $\bar{E}(k,w)$ if $N\to\infty$. In order to see this behavior, we write the precedent equation as follows

$$S_N(k,w) = \int_0^\infty \frac{xe^{-x}}{k(1-w)+wx} \, dx - \frac{w^{N+1}}{k} \int_0^\infty xe^{-x} \, \frac{(1-x/k)^{N+1}}{1-w(1-x/k)} \, dx =$$

$$= \bar{E}(k,w) - R_N(k,w) \tag{51.30}$$

where R_N is the remainder to be examined:

$$R_N(k,w) = \frac{w^{N+1}}{k} \int_0^\infty xe^{-x} \, \frac{(1-x/k)^{N+1}}{1-w(1-x/k)} \, dx =$$

$$= w^{N+1} \int_0^\infty xe^{-x} \, \frac{(1-x/k)^{N+1}}{k+w(x-k)} \, dx \quad . \tag{51.31}$$

Due to Eq. (51.30), the convergence analysis of $S_N(k,w)$ when $\lambda, N\to\infty$ turns into the study of $R_N(k,1)$ at the limit $N\to\infty$. The discussion is made in a similar fashion as done for $\bar{E}^{(N)}$. Thus, we have

$$R_N(k,1) = A_1 + A_2 \tag{51.32a}$$

$$A_1 = \int_0^k e^{-x} \, (1-\tfrac{x}{k})^{N+1} \, dx \; ; \; A_2 = \int_k^\infty e^{-x} (1-\tfrac{x}{k})^{N+1} \, dx \quad . \tag{51.32b}$$

It is found at once the following bound for A_1:

$$A_1 \leq \int_0^k e^{-x} e^{-x(N+1)/k}\, dx \leq \int_0^\infty e^{-x}\left(\frac{N+1}{k} + 1\right) dx = \frac{k}{N+1+k} \qquad (51.33a)$$

where the equality is valid when $N,k\to\infty$. Similarly, it is found for A_2

$$A_2 = e^{-k} \int_0^\infty e^{-y}\left(-\frac{y}{k}\right)^{N+1} dy = \left(-\frac{1}{k}\right)^{N+1} e^{-k}(N+1)! \quad , \qquad (51.33b)$$

and the application of (51.22) permits one to write the remainder as

$$R_N(k,1) \leq \left(-\frac{1}{N^r}\right)^{N+1} \delta^{-(N+1)} e^{-\delta N^r} (N+1)! + \frac{\delta N^r}{N+1+\delta N^r} \quad . \qquad (51.34)$$

When $N\to\infty$, the first term at the r.h.s. in (51.34) is infinite if $r<1$, and null when $r\geq 1$. This result find for the remainder that

$$\lim_{N\to\infty} R_N(k,1) = \frac{\delta}{1+\delta} \text{ if } r = 1 \quad , \qquad (51.35a)$$

$$\lim_{N\to\infty} R_N(k,1) = 1 \quad \text{if} \quad r>1 \quad . \qquad (51.35b)$$

Eq. (51.35) is important since it shows that R_N is not zero when $w = 1$ $(1/\lambda\to 0)$ and therefore $S_N(k,w)$ does not converge to $\bar{E}(k,w)$ when $N\to\infty$. Notice that, since $\delta>0$, the smallest remainder occurs when $r = 1$, that is to say, when the order dependence is setted by the scaling law ($\alpha=-1$ in Eq. (49.37)). The situation found here is similar to that one discussed in §.47 for the geometrical series, in the sense that order-dependent sequences with a linear correlation k vs N do not converge to the exact result. However, we have found a new fact: considering a function with $\alpha=-1$, and an asymptotically divergent power series expansion about $\alpha=0$, the sequences like $k=\delta N$ are those converging nearest the exact result.

According to the FM, the δ parameter must be found first determining the $S_N(k,1)$ sequences of IP and SP and then to fit them linearly with N. The result (51.35a) makes certain that the introduced error will be less when the slope δ decreases.

Now, we have all the necessary elements to find the $S_N(k,w)$ value when $N\to\infty$. In order to take the limit $N\to\infty$ in (51.31), we notice that from Eq. (51.18c) it follows that

$$\ln w = - \ln(1+\frac{1}{\lambda k}) \simeq - \frac{1}{\lambda k} \text{ when } k>>1 \text{ and } \lambda>1 \qquad (51.36)$$

which enables us to obtain the following result with the help of (51.22) (r = 1):

$$\lim_{N\to\infty} w^{N+1} = e^{-1/\delta\lambda} \qquad (51.37)$$

In addition to this, we know that

$$\lim_{N\to\infty} \{k+w(x-k)\} = \lim_{N\to\infty} \{ \frac{\delta N(1+\lambda x)}{1+\lambda\delta N}\} = \frac{1}{\lambda} + x \qquad (51.38a)$$

and

$$\lim_{N\to\infty} (1-\frac{x}{k})^{N+1} = \lim_{N\to\infty} (1-\frac{x}{\delta N})^{N+1} = e^{-x/\delta} \qquad (51.38b)$$

The substitution of (51.37) and (51.38) into (51.30) yields

$$\lim_{N\to\infty} S_N(k,w) = \bar{E}(k,w) -e^{-1/\delta\lambda} \int_0^\infty \frac{xe^{-x(1+1/\delta)}}{x+1/\lambda} dx \qquad (51.39)$$

and the change of variables $y = (\delta+1)x/\delta$ turns (51.39a) into

$$\lim_{N\to\infty} S_N(k,w) = \bar{E}(k,w) - \lambda e^{-1/\delta\lambda} (\frac{\delta}{\delta+1})^2 \int_0^\infty \frac{ye^{-y}}{1+ \frac{\lambda\delta}{1+\delta} y} dy =$$

$$- \bar{E}(k,w) - \lambda e^{-1/\delta\lambda} \left(\frac{\delta}{1+\delta}\right)^2 E(1,\lambda\delta/(1+\delta)) \qquad (51.40)$$

Finally, Eq. (44.8b) with $\beta=-1$ (See Eq. (51.11)) allows us to find the FM estimate for $E(1,\lambda)$:

$$\lim_{N\to\infty} SE_N = E(1,\lambda)-e^{-1/\delta\lambda} \left(\frac{\delta}{1+\delta}\right)^2 E(1,\delta\lambda/(1+\delta)) \qquad (51.41)$$

The remainder in Eq. (51.41) is not null for $\lambda>0$ and for this reason the FM permits one to construct a sequence converging to a lower bound for $E(1,\lambda)$. This sequence is determined by an order dependent mapping where k is proportional to N. The direct application of the FM and the Sensitivity Rules lead to the same result.

Before proceeding to verify numerically our predictions, we show that it is possible to draw identical conclusions regarding the remainder $R_N(k,1)$ by means of a totally algebraic treatment of the FM equations

The application of Eq. (44.8a) to (51.16) leads us to

$$E(1,\lambda) = k^{-1}(1-w)^{-1} \bar{E}(k,w) = k^{-1}(1-w)^{-1} \sum_{n=0}^{\infty} \bar{E}^{(n)} w^n \qquad (51.42)$$

where according to Eq. (44.18)

$$\bar{E}^{(n)} = \sum_{j=0}^{n} \frac{n!}{(n-j)!j!} E^{(j)} k^{-(1+j)} \qquad (51.43)$$

On introducing the coefficients (51.15) into (51.43) and setting $k=\delta N$, we have

$$\bar{E}^{(n)} = \frac{1}{k} \sum_{j=0}^{n} \frac{n!(j+1)}{(n-j)!} \left(-\frac{1}{\delta N}\right)^j = \frac{1}{k} \{1- \frac{2n}{\delta N} + \frac{3n(n-1)}{\delta^2 N^2} - \ldots\} \qquad (51.44a)$$

The partial sum for N>>1 is

$$\sum_{n=0}^{N} \bar{E}^{(n)} = \frac{1}{k} \{N - \frac{2}{\delta N} (\frac{N2}{2}) + \frac{3}{\delta^2 N^2} (\frac{N^3}{3}) - \ldots\} =$$

$$= \{ \frac{1}{\delta} - \frac{1}{\delta}2 + \frac{1}{\delta}3 - \ldots\} \qquad . \qquad (51.44b)$$

Finally

$$\lim_{N\to\infty} \sum_{n=0}^{N} \bar{E}^{(n)} = - \sum_{n=1}^{\infty} (- \frac{1}{\delta})^n = -(-1 + \frac{1}{1+1/\delta}) = \frac{1}{1+\delta} \qquad (51.45)$$

which leads to (51.40) when $1/\lambda \to 0$.

In order to complete this section, let us verify that the Sensitivity Rules allow to derive the convergent sequence previously obtained. Results corresponding to k_N^S and $S_N(k_N^S,1)$ are shown in Table 15.5 for $N \leq 31$.

Table 15.5: Convergent renormalized sequence for the function (51.16).

N	k_N^S	$S_N(k_N^S,1)$	N	k_N^S	$S_N(k_N^S,1)$
1	2.0000	0.4959	17	6.7794	0.7264
3	2.6258	0.6037	19	7.3594	0.7310
5	3.2371	0.6496	21	7.9377	0.7349
7	3.8392	0.6757	23	8.5145	0.7381
9	4.4349	0.6928	25	9.0901	0.7409
11	5.0238	0.7048	27	9.6646	0.7434
13	5.6131	0.7138	29	10.2381	0.7456
15	6.1975	0.7208	31	10.8107	0.7475

A standard linear regression for the 6 last SP yields

$$k_N^S = (1.91 \pm 0.03) + (0.287 \pm 0.001)N \; ; \; r = 0.99999911 \qquad (51.46)$$

According to the precedent equations, $S_N(k_N^S,1)$ should converge to $1/(1+\delta) \simeq 0.78$ when $N \to \infty$ in agreement with the last approximation in Table 15.5 $S_{31}(k_{31}^S,1) \simeq 0.75$.

It is to be noted that several problems of Physical and Physical Chemistry interest present a situation similar to that discussed in this section, that is, there are functions fulfilling scaling laws which cannot be expanded around $1/\lambda = 0$. Such cases will be discussed in forthcoming chapters.

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