

# Theorems on Estimating Perturbative Coefficients in Quantum Field Theory and Statistical Physics

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We present rigorous proofs for several theorems on using Padé approximants to estimate coefficients in perturbative quantum field theory and statistical physics. As a result, we find new trigonometric and other identities where the estimates based on this approach are exact. We discuss hypergeometric functions, as well as series from both perturbative quantum field theory and statistical physics.

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## 1. INTRODUCTION

Recently, we proposed (Samuel *et al.*, 1993a,b, 1994a; Samuel and Li, 1993, 1994) a method of estimating coefficients in perturbative quantum field theory and statistical physics with error bars for each estimate. The method makes use of Padé approximants and yields a Padé approximant approximation (PAP). There are many good references for Padé approximants, such as Zinn-Justin (1971), Nutall (1970), Baker (1975), Bender and Orzag (1978), Chlouber *et al.* (1992). We begin by defining the Padé approximant

$$[N/M] = \frac{a_0 + a_1x + a_2x^2 + \dots + a_Nx^N}{1 + b_1x + b_2x^2 + b_3x^3 + \dots + b_Mx^M} \quad (1.1)$$

to the series

$$S = S_0 + S_1x + \dots + S_{N+M}x^{N+M} \quad (1.2)$$

where we set

$$[N/M] = S + O(x^{N+M+1}) \quad (1.3)$$

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We have written a computer program that solves equation (1.3) numerically and then predicts the coefficient of the next term  $S_{N+M+1}$ . It works for arbitrary  $N$  and  $M$ . Furthermore, we have derived algebraic formulas for the  $[N/1]$ ,  $[N/2]$ ,  $[N/3]$ ,  $[N/4]$ ,  $[N/5]$ , and  $[N/6]$  PAPs, where  $N$  is arbitrary.

To illustrate the method, consider the simple example

$$\frac{\ln(1+x)}{x} = 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{C} \tag{1.4}$$

We write the  $[1/1]$  Padé as

$$[1/1] = \frac{a_0 + a_1x}{1 + b_1x} \tag{1.5}$$

It is easy to show that  $a_0 = 1$ ,  $b_1 = 2/3$ ,  $a_1 = 1/6$ , and  $C = 9/2$ . We can see that the prediction for  $C$  is close to the correct value  $C = 4$ . For  $x = 1$ , we get  $[1/1] = 7/10$ , close to the correct result,  $\ln 2 = 0.6931$ . This is much better than the partial sum

$$1 - \frac{1}{2} + \frac{1}{3} = \frac{5}{6} = 0.8333 \tag{1.6}$$

By going to higher order, it is easy to show that

$$[1/2] = \frac{1 + x/2}{1 + x + x^2/6} \tag{1.7}$$

and for  $x = 1$  we obtain

$$m[1/2] = \frac{9}{13} = 0.6923 \tag{1.8}$$

very close to  $\ln 2$ . The PAP is  $7/36 = 0.1944$ , very close to the correct value of  $1/5$ .

The error bars are obtained by taking the reciprocals

$$r_n = \frac{1}{S_n} \tag{1.9}$$

and finding the PAP for  $r_{n+1}$ , and then taking the reciprocal. Then we consider the differences

$$t_n = r_{n+1} - r_n \tag{1.10}$$

and find the PAP for  $t_n$ . We then have

$$r_{n+1} = r_n + t_n \tag{1.11}$$

and then take the reciprocal

$$S_{n+1} = \frac{1}{r_{n+1}} \tag{1.12}$$

Our error bar is calculated from the difference between the results from equations (1.9) and (1.12).

## 2. THEOREMS

We consider the general series

$$S = \sum_n S_n x^n \tag{2.1}$$

*Theorem A. Sums of Geometric Series.* If  $S_n$  is a sum of  $M$  geometric series, then the  $[N/M]$  PAP for  $N \geq M - 1$  is exact.

*Proof.* For  $M = 2$ ,

$$S_n = ar^n + bs^n \tag{2.2}$$

and

$$S = \sum_{n=0}^{\infty} S_n x^n = \frac{a}{1 - rx} + \frac{b}{1 - sx} \tag{2.3}$$

so that

$$S = \frac{(a + b) - (as + br)x}{(1 - rx)(1 - sx)} \tag{2.4}$$

and the  $[1/2]$  and higher PAPs are exact.

To prove the general case we use mathematical induction. Assume that the theorem is true for the  $[M - 1/M]$  PAP. Now for  $M \rightarrow M + 1$ , we have

$$\frac{P_{M-1}}{Q_M} + \frac{g}{1 - ax} = \frac{P_{M-1} + gQ_M}{Q_M(1 - ax)} \tag{2.5}$$

and the  $[M/M + 1]$  PAP is exact. Here

$$S_n = ar^n + bs^n + \dots + gw^n \tag{2.6}$$

and  $P_M$  and  $Q_M$  are polynomials of degree  $M$ .

*Theorem B. Signs of Geometric Series.* For

$$S_n = (-1)^n c_m ar^n \tag{2.7}$$

the  $[m - 1/m]$  PAP is exact.

*Proof.* The proof is easily obtained by recognizing that the series in equation (2.7) is just a sum of geometric series and by next using Theorem A.

*Theorem C. A Sufficient Condition for PAPs to Be Accurate.* If we define

$$g(n) = \frac{d^2 \ln S_n}{dn^2} \tag{2.8}$$

then a sufficient (but not necessary) condition for the PAPs to be accurate is

$$\lim_{n \rightarrow \infty} g(n) = 0 \tag{2.9}$$

*Proof.* We define

$$A_n \equiv 1 + \epsilon_n \equiv \frac{S_n S_{n+2}}{(S_{n+1})^2} \tag{2.10}$$

and hence

$$A_n = 1 + \epsilon_n = e^{g(n)} \tag{2.11}$$

The percent error is expressible in terms of the  $\epsilon_n$  and if  $g(n) \rightarrow 0$ , then  $\epsilon_n \rightarrow 0$  and the PAP is accurate.

*Theorem D. A Generalization of Theorem C.* If, in addition to the conditions of Theorem C for  $S_n$  we generalize to a series

$$T = \sum_n T_n x^n \tag{2.12}$$

where

$$T_n = (-1)^n C_m S_n \tag{2.13}$$

then the  $[m - 1/m]$  and higher PAPs will be accurate.

*Proof.* We have

$$A'_n = 1 + \epsilon'_n = (-1)^n C_{m-2} A_n \tag{2.14}$$

where  $A_n$  is given by equation (24). Then we use Theorems B and C to prove Theorem D. For further details, see Samuel *et al.* (1993b).

*Theorem E. Polynomials of the nth Degree.* For  $S_n = P_n$  where  $P_n$  is a polynomial of degree  $n$ , the  $[N/M]$  PAPs are exact, where  $M = n + 1$  and  $N \geq M - 1$ .

*Proof.* By differentiating

$$S = \sum_n x^n = (1 - x)^{-1} \tag{2.15}$$

and multiplying by  $x$ , we obtain

$$\sum_n (an + b)x^n = \frac{(a - b)x + b}{(1 - x)^2} \tag{2.16}$$

and the  $[N/2]$  is exact for  $N \geq 1$ . Now by induction we can easily obtain the desired result.

It should be emphasized that in all cases once the  $[N/M]$  PAPs are exact for  $N \geq M - 1$ , the results remain exact for all higher-order PAPs  $[N'/M']$  for  $M' > M$  and  $N' > M' - 1$ .

### 3. SOME NEW TRIGONOMETRIC IDENTITIES

If we consider the series given by

$$S_n = \sin[(n + 1)\theta + \delta] \tag{3.1}$$

where  $\theta$  and  $\delta$  are arbitrary, we will prove that the  $[N/M]$  PAPs are exact for  $M \geq 2$  and  $N \geq M - 1$ . This leads to new trigonometric identities corresponding to each of the  $[N/2]$ ,  $[N/3]$ ,  $[N/4]$ , etc., PAPs.

From equation (3.1) it can easily be shown that

$$\begin{aligned} S &= \sum_{n=0}^{\infty} S_n x^n \\ &= \frac{x \cos(\theta + \delta) \sin \theta + \sin(\theta + \delta) (1 - x \cos \theta)}{1 - 2x \cos \theta + x^2} \end{aligned} \tag{3.2}$$

Hence the  $[N/M]$  PAPs are exact for  $M \geq 2$ ,  $N \geq M - 1$ . With  $\delta = 0$ , equation (3.2) becomes

$$S = \frac{\sin \theta}{1 + x^2 - 2x \cos \theta} \tag{3.3}$$

and hence the  $[0/2]$  PAP is exact.

Similarly, for

$$S_n = \cos[(n + 1)\theta + \delta] \tag{3.4}$$

we can obtain

$$S = \frac{\cos(\theta + \delta) (1 - x \cos \theta) - x \sin(\theta + \delta) \sin \theta}{1 - 2x \cos \theta + x^2} \tag{3.5}$$

In this case, however, if we set  $\delta = 0$ , we obtain

$$S = \frac{\cos \theta - x}{1 - 2x \cos \theta + x^2} \tag{3.6}$$

and the  $[0/2]$  PAP is not exact!

Now, for each  $[N/M]$  PAP that is exact we find a trigonometric identity. We begin with  $M = 2$ . The  $[1/2]$  PAP is given by  $S_4 = N/D$ , where

$$N = 2S_1S_2S_3 - S_0S_3^2 - S_2^3 \quad (3.7)$$

and

$$D = S_1^2 - S_0S_2 \quad (3.8)$$

with the  $S_n$  given by equation (3.1). Thus we have the identity

$$N - S_4D \equiv 0 \quad (3.9)$$

which becomes

$$\begin{aligned} & 2 \sin(2\theta + \delta) \sin(3\theta + \delta) \sin(4\theta + \delta) \\ & - \sin(\theta + \delta) \sin^2(4\theta + \delta) - \sin^3(3\theta + \delta) \\ & - \sin(5\theta + \delta) [\sin^2(2\theta + \delta) - \sin(\theta + \delta) \sin(3\theta + \delta)] = 0 \end{aligned} \quad (3.10)$$

Now one can step up in  $n$ ,  $S_n \rightarrow S_{n+1}$ , and obtain another identity. This procedure can be repeated indefinitely. One can also step down in  $n$ ,  $S_n \rightarrow S_{n-1}$ , where we set  $S_{-1} = 0$ . This gives a simpler identity, which can be obtained from simple known identities, for the  $[0/2]$  PAP. But we must set  $\delta = k\pi$ ,  $k = 0, 1, 2, \dots$ , yielding

$$2 \sin\theta \sin(2\theta) \sin(3\theta) - \sin^3(2\theta) - \sin(4\theta) \sin^2\theta = 0 \quad (3.11)$$

One can also use equation (31) to obtain the same identities for  $\cos[(n + 1)\theta + \delta]$ . However, in this case there is no  $[0/2]$  identity for  $\delta = 0$ .

We now turn to  $M = 3$ . The  $[2/3]$  PAP is given by

$$S_6 = A/B \quad (3.12)$$

where

$$\begin{aligned} A = & 2S_2^2S_3S_5 - 2S_1S_3^2S_5 + 2S_0S_3S_4S_5 \\ & - 2S_1S_2S_4S_5 + S_1^2S_5^2 - S_0S_2S_5^2 + S_2^2S_4^2 \\ & - 3S_2S_3^2S_4 + 2S_1S_3S_4^2 - S_0S_4^3 + S_4^4 \end{aligned} \quad (3.13)$$

and

$$B = S_2^3 - 2S_1S_2S_3 + S_0S_3^2 - S_0S_2S_4 + S_1^2S_4 \quad (3.14)$$

Again we use equation (3.1) and (3.4), but this time there are two identities in each case

$$A = 0 \quad \text{and} \quad B = 0 \quad (3.15)$$

The first part of equation (3.15) yields new identities, but the second part gives only previous identities for  $M = 2$ . This is in accordance with a theorem presented in an earlier paper (Samuel *et al.*, 1993b). We can again step up in  $n$ ,  $S_n \rightarrow S_{n+1}$ , and obtain more identities for both  $\sin[(n + 1)\theta + \delta]$  and  $\cos[(n + 1)\theta + \delta]$ . This process may be repeated as many times as desired. Now we may very easily also step down in  $n$ ,  $S_n \rightarrow S_{n-1}$ , where we set  $S_{-1} = 0$ . This gives identities for the [1/3]. In this case the identity obtained results from

$$A - BS_6 = 0 \tag{3.16}$$

for both sine and cosine, with  $\delta \neq n\pi$ . For the sine case, if  $\delta = k\pi$ , we obtain

$$A = 0 \quad \text{and} \quad B = 0 \tag{3.17}$$

If we step down once more to the [0/3] PAP and set  $\delta = k\pi$ , then we obtain an identity for sine, but not for cosine.

Although this process can be continued indefinitely for  $M = 4, 5, 6, \dots$ , the formulas become increasingly complicated, as will soon be seen. So we present results for only one more value of  $M$ , namely  $M = 4$ . The [3/4] PAP is given by

$$S_8 = C/D \tag{3.18}$$

where

$$\begin{aligned} C = & 2(2S_2S_3S_4^2S_7 - S_3^3S_4S_7 - S_1S_4^3S_7 \\ & - S_2^2S_4S_5S_7 + S_1S_3S_4S_5S_7 + S_3^2S_4^2S_6 + 2S_1S_4^2S_5S_6 \\ & + S_2^2S_4S_6^2 - S_1S_3S_4S_6^2 - S_2S_3S_4S_5S_6 - S_2S_4^3S_6 \\ & + S_3^2S_4S_5^2 + S_2S_4^2S_5^2 - 2S_3S_4^3S_5 - S_1S_4S_5^3 + S_2S_3^2S_5S_7 \\ & + S_0S_4^2S_5S_7 + S_1S_2S_5^2S_7 - S_0S_3S_5^2S_7 - S_2^2S_4S_5S_7 \\ & - S_1S_3S_4S_5S_7 - S_2^2S_3S_6S_7 - S_0S_3S_4S_6S_7 - S_1^2S_5S_6S_7 \\ & + S_0S_2S_5S_6S_7 + S_1S_2S_4S_6S_7 + S_1S_3^2S_6S_7 - S_1S_2S_3S_7^2 \\ & - S_3^3S_5S_6 - S_1S_3S_4S_6^2 - S_1S_2S_5S_6^2 + S_1S_3S_5^2S_6 \\ & + S_0S_3S_5S_6^2 - S_2S_3S_5^3) - 3S_0S_4S_5^2S_6 + S_2^2S_7^2 + S_0S_3^2S_7^2 \\ & + S_1^2S_4S_7^2 - S_0S_2S_4S_7^2 + S_2S_3^2S_6^2 + S_1^2S_6^3 - S_0S_2S_6^3 \\ & + S_3^2S_4S_5^2 + S_2^2S_5^2S_6 + S_4^5 + S_2S_4^2S_5^2 + S_3^2S_4^2S_6 \\ & - S_2S_4^3S_6 + S_0S_4^2S_6^2 + S_0S_5^4 \end{aligned} \tag{3.19}$$

and

$$\begin{aligned}
 D = & 2(S_1 S_3^2 S_5 + S_1 S_2 S_4 S_5 - S_1 S_3 S_4^2 \\
 & - S_2^2 S_3 S_5 - S_1 S_2 S_3 S_6 - S_0 S_3 S_4 S_5) + 3S_2 S_3^2 S_4 \\
 & - S_3^4 - S_1^2 S_5^2 + S_1^2 S_4 S_6 + S_0 S_4^3 + S_0 S_2 S_3^2 \\
 & + S_0 S_3^2 S_6 - S_0 S_2 S_4 S_6 + S_2^3 S_6 - S_2^2 S_4^2
 \end{aligned} \tag{3.20}$$

The identities for the [3/4] PAP are

$$C = 0 \quad \text{and} \quad D = 0 \tag{3.21}$$

for arbitrary  $\delta$  in both the sine and cosine cases. Again we may step up  $S_n \rightarrow S_{n+1}$ , etc., and obtain new identities. We may also step down to the [2/4] PAP. For the [1/4] PAP the identity is obtained for arbitrary  $\delta$  from

$$C - DS = 0 \tag{3.22}$$

For  $\delta = k\pi$  we obtain for the sine case the identities

$$C = 0 \quad \text{and} \quad D = 0 \tag{3.23}$$

For the [0/4], for  $\delta = k\pi$ , sine works, but not cosine.

We believe these identities are new, except for the [0/2] PAP. We would be interested in hearing from anyone who believes any of these identities are already known.

#### 4. THE GENERALIZED HYPERGEOMETRIC FUNCTION

The hypergeometric function  ${}_kF_m$  represents a large number of elementary functions. Thus we can consider PAPs for many functions at once. We will see that the PAPs are accurate for arbitrary  $k$  and  $m$  and a large number of parameters  $a, b, c, \dots$ . For many examples of how numerous mathematical functions can be expressed in terms of the hypergeometric function  ${}_2F_1$  or the confluent hypergeometric function  ${}_1F_1$  see, for example, the books by Arfken (1985), Abramowitz and Stegun (1964), and Gradshteyn and Ryzhik (1980).

Consider the hypergeometric series given by

$$S_n = \frac{(a)_n (b)_n}{(c)_n n!} \tag{4.1}$$

where

$$(a)_n = a(a + 1) \dots (a + n + 1) \tag{4.2}$$



and hence

$${}_2F_1(a, b, c; x) = \sum_{n=0}^{\infty} S_n x^n \tag{4.3}$$

For the  $[N/2]$  PAP the percentage error is given by  $100p$ , where

$$p = \frac{\epsilon_N^2/\epsilon_{N-1} - \epsilon_{N+1}(1 + \epsilon_N)^2}{(1 + \epsilon_N)^2(1 + \epsilon_{N+1})}; \quad N \geq 1 \tag{4.4}$$

It can be shown for the  ${}_2F_1$  hypergeometric function that

$$p \sim \frac{-2B(1 + B)}{N^4} \tag{4.5}$$

where

$$B = c + 1 - a - b \tag{4.6}$$

and hence the PAPs quickly become accurate as  $N \rightarrow \infty$ . For  ${}_1F_1(a, c; x)$

$$p \sim +\frac{2}{N^2} \tag{4.7}$$

and for  ${}_2F_0(a, b, c; x)$

$$p \sim -\frac{2}{N^2} \tag{4.8}$$

For the general case  ${}_kF_m$ , if  $k \neq m + 1$ ,

$$p \sim \frac{2A}{N^2} \tag{4.9}$$

where

$$A = k - (m + 1) \tag{4.10}$$

and if  $k = m + 1$ , then

$$p \sim \frac{-2B(1 + B)}{N^4} \tag{4.11}$$

where

$$B = 2 + k^2 - 2k + m - km + \sum_{i=1}^m c_i - \sum_{i=1}^k a_i \tag{4.12}$$

In general if

$$\epsilon_n \sim A/N \quad (4.13)$$

then

$$p \sim -2A^2/N^2 \quad (4.14)$$

and if

$$\epsilon_n \sim B/N^2 \quad (4.15)$$

then

$$p \sim -2B(1 + B)/N^4 \quad (4.16)$$

To check the behavior for  $M \neq 2$  we have written a computer program that scans over  $a$ ,  $b$ , and  $c$  values (skipping over integers) and evaluates the corresponding PAPs. The parameters  $a$ ,  $b$ , and  $c$  vary from  $-5.0$  to  $5.0$  in steps of  $0.125$ . For each  $[N/M]$  PAP, the fractional error  $p$  is evaluated, and the maximum and minimum values of  $p$  listed as TESTMAX and TESTMIN, respectively. The results for  ${}_2F_1$ ,  ${}_1F_1$ , and  ${}_2F_0$  are presented in Tables I–III, respectively. It can be seen that the TESTMIN and TESTMAX values decrease rapidly in going to progressively higher order. We have listed only diagonal PAPs, but other Padé's were also computed and gave very good results.

Table I. Padé Estimates for  ${}_2F_1$

$[N/M]$	TESTMIN	TESTMAX
[4/4]	$0.649 \times 10^{-8}$	0.649
[5/5]	$0.105 \times 10^{-9}$	34.0
[6/6]	$0.103 \times 10^{-11}$	2.57
[7/7]	$0.100 \times 10^{-13}$	7.0
[8/8]	$0.107 \times 10^{-15}$	0.494
[9/9]	$0.136 \times 10^{-17}$	$0.687 \times 10^{-2}$
[10/10]	$0.173 \times 10^{-19}$	$0.332 \times 10^{-3}$
[11/11]	$0.284 \times 10^{-21}$	$0.151 \times 10^{-4}$
[12/12]	$0.442 \times 10^{-23}$	$0.215 \times 10^{-5}$
[13/13]	$0.757 \times 10^{-25}$	$0.294 \times 10^{-6}$
[14/14]	$0.151 \times 10^{-26}$	$0.386 \times 10^{-7}$
[15/15]	$0.652 \times 10^{-30}$	$0.492 \times 10^{-8}$
[16/16]	$0.197 \times 10^{-29}$	$0.611 \times 10^{-9}$
[17/17]	$0.705 \times 10^{-30}$	$0.720 \times 10^{-10}$
[18/18]	$0.192 \times 10^{-29}$	$0.847 \times 10^{-11}$

Table II. Padé Estimates for  ${}_1F_1$ 

$[N/M]$	TESTMIN	TESTMAX
[4/4]	$0.536 \times 10^{-5}$	$0.246 \times 10^{-6}$
[5/5]	$0.170 \times 10^{-6}$	6.721
[6/6]	$0.195 \times 10^{-6}$	35.4
[7/7]	$0.251 \times 10^{-6}$	4.56
[8/8]	$0.124 \times 10^{-7}$	0.456
[9/9]	$0.878 \times 10^{-8}$	$0.102 \times 10^{-1}$
[10/10]	$0.835 \times 10^{-9}$	$0.114 \times 10^{-2}$
[11/11]	$0.168 \times 10^{-8}$	$0.697 \times 10^{-3}$
[12/12]	$0.148 \times 10^{-9}$	$0.260 \times 10^{-3}$
[13/13]	$0.394 \times 10^{-10}$	$0.270 \times 10^{-3}$
[14/14]	$0.419 \times 10^{-11}$	$0.676 \times 10^{-5}$
[15/15]	$0.157 \times 10^{-11}$	$0.119 \times 10^{-5}$
[16/16]	$0.530 \times 10^{-13}$	$0.844 \times 10^{-6}$
[17/17]	$0.393 \times 10^{-13}$	$0.121 \times 10^{-6}$
[18/18]	$0.984 \times 10^{-14}$	$0.201 \times 10^{-7}$
[19/19]	$0.259 \times 10^{-14}$	$0.217 \times 10^{-8}$
[20/20]	$0.158 \times 10^{-14}$	$0.128 \times 10^{-8}$

Table III. Padé Estimates for  ${}_2F_0$ 

$[N/M]$	TESTMIN	TESTMAX
[4/4]	$0.146 \times 10^{-4}$	127.3
[5/5]	$0.118 \times 10^{-4}$	45.3
[6/6]	$0.458 \times 10^{-6}$	0.304
[7/7]	$0.259 \times 10^{-5}$	3.00
[8/8]	$0.986 \times 10^{-8}$	$0.307 \times 10^{-1}$
[9/9]	$0.262 \times 10^{-8}$	$0.247 \times 10^{-1}$
[9/10]	$0.528 \times 10^{-8}$	$0.227 \times 10^{-1}$
[10/9]	$0.572 \times 10^{-9}$	$0.298 \times 10^{-2}$
[10/10]	$0.590 \times 10^{-8}$	$0.152 \times 10^{-1}$
[11/11]	$0.165 \times 10^{-8}$	$0.774 \times 10^{-1}$
[13/13]	$0.132 \times 10^{-10}$	$0.573 \times 10^{-4}$
[13/14]	$0.298 \times 10^{-10}$	$0.227 \times 10^{-3}$
[14/13]	$0.214 \times 10^{-10}$	$0.776 \times 10^{-3}$
[16/16]	$0.136 \times 10^{-11}$	$0.151 \times 10^{-5}$
[17/17]	$0.377 \times 10^{-13}$	$0.105 \times 10^{-6}$
[18/18]	$0.272 \times 10^{-13}$	$0.275 \times 10^{-7}$
[19/19]	$0.349 \times 10^{-14}$	$0.729 \times 10^{-8}$
[20/20]	$0.296 \times 10^{-16}$	$0.198 \times 10^{-8}$

### 5. OTHER EXAMPLES OF EXACT PAPs

Other examples can be found in which PAPs are exact. Any series whose sum is a rational fraction of two polynomials

$$S = \sum_{n=0}^{\infty} S_n x^n = \frac{P_{N_0}(x)}{Q_{M_0}(x)} \tag{5.1}$$

will be exact for the  $[N/M]$  PAP where  $N \geq N_0$  and  $M \geq M_0$ . Some examples include

$$S_n = (2n + 1); \quad N_0 = 1, \quad M_0 = 2 \tag{5.2}$$

$$S_n = (n + 1)^2; \quad N_0 = 1, \quad M_0 = 3 \tag{5.3}$$

$$S_n = (2n + 1)^2; \quad N_0 = 2, \quad M_0 = 3 \tag{5.4}$$

$$S_n = (a + nd); \quad N_0 = 1, \quad M_0 = 2 \tag{5.5}$$

$$S_n = (n + 1); \quad N_0 = 0, \quad M_0 = 2 \tag{5.6}$$

$$S_{n+1} - S_n = (n + 2), \quad S_0 = 1; \quad N_0 = 0, \quad M_0 = 3 \tag{5.7}$$

and

$$S_n = 1; \quad N_0 = 0, \quad M_0 = 1 \tag{5.8}$$

### 6. NONSINGLET MOMENTS OF DEEP INELASTIC STRUCTURE FUNCTIONS IN QCD

In this section we make use of some recent results of Larin *et al.* (1993). They calculated the next-to-next leading QCD approximations for nonsinglet moments of deep inelastic structure functions, in the leading twist approximation, for the moments  $N = 2, 4, 6, 8$  of the nonsinglet deep inelastic structure function  $F_L$ . They calculated the three-loop anomalous dimensions of the corresponding nonsinglet operators and the three-loop coefficient functions of the structure factor  $F_L$ , in the leading twist and massless quark approximation.

We present our results in Tables IV–XI. In each case, we estimate the  $O(\alpha_s^3)$  coefficient and compare our estimate with the Larin *et al.* result. We neglect the term that depends on the sum of the quark charges  $\sum q_f$ , since the term is small in all cases of interest. We present our results for  $N_f = 3, 4, 5$ , where  $N_f$  is the number of quark flavors. We then present our estimates for the next (unknown)  $O(\alpha_s^4)$  coefficients, in each case.

In Table IV we present results for  $C_{L,2}$ . It is seen that for  $N_f = 3, 4, 5$  our estimates are within the error bars for the  $O(\alpha_s^3)$  terms and we estimate the next (unknown)  $O(\alpha_s^4)$  terms. Table V shows the results for  $C_{L,4}$ , Table VI for  $C_{L,6}$ , and Table VII for  $C_{L,8}$ .

**Table IV.** Padé Estimates for  $C_{L,2}$

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
1,046	1,046	2,230	1,184
82,812	205,498	—	—
$N_f = 4$			
837	837	2,313	1,476
82,233	32,915	—	—
$N_f = 5$			
652	652	2,420	1,768
80,203	13,522	—	—

**Table V.** Padé Estimates for  $C_{L,4}$

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
1,376	668	1,473	137
56,946	29,021	—	—
$N_f = 4$			
1,106	553	1,166	60
39,468	19,846	—	—
$N_f = 5$			
897	449	881	16
25,076	4,004	—	—

**Table VI.** Padé Estimates for  $C_{L,6}$

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
2,305	1,153	1,433	872
41,989	17,795	—	—
$N_f = 4$			
2,018	1,009	1,159	859
27,443	12,654	—	—
$N_f = 5$			
1,750	875	905	845
15,894	8,434	—	—

Table VII. Padé Estimates for  $C_{L,8}$ 

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
1,437	719	1,985	548
124,711	78,967	—	—
$N_f = 4$			
1,226	613	2,043	817
130,095	139,494	—	—
$N_f = 5$			
1,031	516	2,118	1,087
133,699	814,125	—	—

Table VIII. Padé Estimates for  $\gamma_2$ 

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
424	212	448	24
5,159	2,270	—	—
$N_f = 4$			
358	179	306	52
2,607	636	—	—
$N_f = 5$			
298	149	162	136
677	238	—	—

Table IX. Padé Estimates for  $\gamma_4$ 

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
636	318	762	126
8,606	3,146	—	—
$N_f = 4$			
517	259	503	14
4,953	387	—	—
$N_f = 5$			
410	205	239	175
954	297	—	—

Table X. Padé Estimates for  $\gamma_6$ 

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
744	372	946	202
10,676	4,001	—	—
$N_f = 4$			
596	298	621	25
5,245	1,266	—	—
$N_f = 5$			
464	232	290	174
1,201	348	—	—

Table XI. Padé Estimates for  $\gamma_8$ 

Estimate	Error	Exact	Estimate - Exact
$N_f = 3$			
833	417	1,081	248
12,225	4,629	—	—
$N_f = 4$			
662	331	709	47
6,018	2,552	—	—
$N_f = 5$			
510	255	330	180
1,401	393	—	—

In Tables VIII–XI we present our results for the anomalous dimensions  $\gamma_2$ ,  $\gamma_4$ ,  $\gamma_6$ , and  $\gamma_8$ . Here again, in each case our estimates are within the error bars of the Larin *et al.* results for  $O(\alpha_s^3)$  and we estimate the next (unknown)  $O(\alpha_s^4)$  term. For further details on how we obtain our error bars, see Samuel (1994).

## 7. EXAMPLES FROM STATISTICAL PHYSICS

In this section we consider two examples (Domb, 1974) from statistical physics. They are the low-temperature ferromagnetic susceptibility coefficients in the Ising model. Table XII gives the results for the honey-combed (hc) lattice and Table XIII gives the results for the square (sq) lattice.

It can be seen that the results are excellent and that the percent error decreases in going to higher order. In all cases the estimates are within  $2\sigma$  of the exact results for the known coefficients, and the next (unknown)

**Table XII.** Padé Estimates for the Low-Temperature Ferromagnetic Susceptibility Coefficients in the Ising Model (hc Lattice)

Estimate	Error	Exact	Estimate - Exact
8,749	818	8,792	43
35,682	120	35,622	60
143,333	447	143,079	254
569,470	950	570,830	1,360
2,264,740	631	2,264,649	91
8,942,853	2,031	8,942,436	417
35,159,776	8,724	35,169,616	9,840
137,838,225	5,787	137,839,308	1,083
538,596,320	10,430	—	—

**Table XIII.** Padé Estimates for the Low-Temperature Ferromagnetic Susceptibility Coefficients in the Ising Model (sq Lattice)

Estimate	Error	Exact	Estimate - Exact
449	138	416	33
2,715	830	2,791	76
18,699	1,592	18,296	403
118,069	35,392	118,016	53
751,928	146	752,008	80
$4,747 \times 10^3$	$1,410 \times 10^3$	$4,746 \times 10^3$	$O(10^3)$
$2,973 \times 10^4$	$721 \times 10^4$	$2973 \times 10^4$	$O(10^3)$
$18,502 \times 10^4$	$5,494 \times 10^4$	—	—

coefficient is predicted. For the hc lattice the estimate is  $538,596,000 \pm 10,500$  and for the square lattice it is  $185,000,000 \pm 55,000,000$ .

## 8. CONCLUSIONS

We have proved several theorems on using Padé approximants to estimate coefficients in perturbative quantum field theory and statistical physics. These theorems give sufficient conditions for the PAP method of estimating the next term in a series expansion to work. In addition, we have presented new trigonometric identities which we obtained as a result of the PAP being exact. We have also considered the generalized hypergeometric function, for which the method works. As a result, many series are dealt with at the same time, since the hypergeometric function can represent many elementary functions merely by changing the parameters.

We have considered several series from QCD. These are for the nonsinglet moments of deep inelastic structure functions. We have also considered



two series from statistical physics. These are the low-temperature ferromagnetic susceptibility coefficients in the Ising model.

In all cases, the method works beautifully. Thus the information needed for estimating the next term in perturbative series is, in fact, contained in the lower-order results.

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## REFERENCES

- Abramowitz, M., and Stegun, I. A. (1964). *Handbook of Mathematical Functions*, U.S. Government Printing Office, Washington, D.C.
- Arfken, G. (1985). *Mathematical Methods of Physics*, Academic Press, New York.
- Baker, Jr., G. A. (1975). *Essentials of Padé Approximants*, Academic Press, New York.
- Bender, C., and Orzag, S. (1978). *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, New York.
- Chlouber, C., Li, G., and Samuel, M. A. (1992). Padé approximants—type I and type II—and their application, Oklahoma State University Research Note 265 (February 1992).
- Domb, C. (1974). Ising model, in *Phase Transitions and Critical Phenomena*, Vol. 3, C. Domb and M. S. Green, eds., Academic Press, New York.
- Gradshteyn, I. S., and Ryzhik, J. M. (1980). *Tables of Integrals, Series, and Products*, Academic Press, New York.
- Larin, S. A., van Ritbergen, T., and Vermaseren, J. A. M. (1993). The next-next-to-leading QCD approximation for nonsinglet moments of deep inelastic structure functions, NIKHEF-H-93-29 (December 1993).
- Nutall, J. (1970). *Journal of Mathematical Analysis*, **31**, 147.
- Samuel, M. A. (1995). On estimating perturbative coefficients in quantum field theory and statistical physics, Oklahoma State University Research Note 290, *International Journal of Theoretical Physics*, **34**, 1113.
- Samuel, M. A., and Li, G. (1994). On the  $R$  and  $R_r$  ratios at the five-loop level of perturbative QCD, *International Journal of Theoretical Physics*, **33**, 2207.
- Samuel, M. A., and Li, G. (1994). *Physics Letters B*, **331**, 114.
- Samuel, M. A., Li, G., and Steinfields, E. (1993a). *Physical Review D*, **48**, 869.

- Samuel, M. A., Li, G., and Steinfields, E. (1993b). On estimating perturbative coefficients in quantum field theory, condensed matter theory, and statistical physics, Oklahoma State University Research Note 278, *Physics Review E*, May (1995).
- Samuel, M. A., Li, G., and Steinfields, E. (1994a). *Physics Letters B*, **323**, 188.
- Samuel, M. A., Li, G., and Steinfields, E. (1994b). *International Journal of Theoretical Physics*, **33**, 1461 (1994).
- Zinn-Justin, J. (1971). *Physics Reports*, **1**, 55.