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Estimating Perturbative Coefficients in High-Energy Physics and Condensed Matter Theory

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Using our method to estimate perturbative coefficients in quantum field theory (QFT), we consider several examples in high-energy physics and condensed matter theory. The results, in all cases, are remarkably good for the known terms. We also predict the values of as yet unknown terms. Moreover, we consider the general convergence properties of asymptotic series in QFT.

Recently we proposed (Samuel *et al.*, 1992, 1993, 1994) a new method to estimate coefficients, in a given order of perturbative quantum field theory (PQFT) without actually evaluating all of the Feynman diagrams in this order.

Our method makes use of Padé approximants (P.A.). We begin by defining the PA (type I):

$$[N, M] = \frac{a_0 + a_1 xt \cdots + a_N x^N}{1 + b_1 xt \cdots + b_M x^M} \tag{1}$$

$$S = S_0 + S_1 x + \cdots + S_{N+M} x^{N+M} \tag{2}$$

where we set

$$[N, M] = S + O(x^{N+M+1}) \tag{3}$$

To illustrate the method, consider the simple example

$$\frac{\ln(1+x)}{x} = 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{c} \tag{4}$$

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We write the (1, 1) Padé as follows:

$$[1, 1] = \frac{a_0 + a_1 x}{1 + b_1 x} \tag{5}$$

It is easy to show that

$$a_0 = 1, \qquad b_1 = 2/3, \qquad a_1 = 1/6, \qquad c = 9/2$$

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

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

One can easily extend this to calculate

$$[1, 2] = \frac{1 + x/2}{1 + x + x^2/6} \tag{7}$$

and, hence, for $x = 1$, we obtain $9/13 = 0.6923$, remarkably close to the correct value, ln 2. For our purposes here, however, we are interested in the estimate for the next coefficient, r_4. It can easily be seen, either directly or from equation III of equations (8) below, that our estimate is

$$r_4 = -\frac{1}{4} + \frac{12}{27} = 0.1944$$

remarkably close to the correct value, $1/5 = 0.2000$.

We have obtained algebraic formulas for the Padé approximant prediction (PAP) for $[N, M]$, where $M = 1, 2, 3, 4, 5$, and 6, for any N. We present here only the first few, due to space limitations:

$$\begin{array}{lll} \text{I} & S_3 = S_2^2/S_1 & [1, 1] \\ & S_4 = S_3^2/S_2 & [2, 1] \\ \text{II} & S_3 = 2S_1 S_2/S_0 - S_1^3/S_0^2 & [0, 2] \\ \text{III} & S_4 = \dfrac{2S_1 S_2 S_3 - S_0 S_3^2 - S_2^3}{S_1^2 - S_0 S_2} & [1, 2] \end{array} \tag{8}$$

where I uses two terms, II three terms, and III four terms. Moreover, we have a computer program which computes the PAP $[N, M]$ for any N and M, by solving the linear equations (1)–(3) numerically. The results from the computer program agree with our formulas in all cases.

Consider first the series

$$[f(y)]^{-1} = 1 + y - y^2 + 3y^3 - 13y^4 + 71y^5 - 461y^6 + 3447y^7 - 29{,}093y^8 \quad (9)$$

where

$$f(y) = \sum_{n=0}^{\infty} (-1)^n n! y^n = {}_2F_0(1; 1; -y) \quad (10)$$

is the Euler series and F is the hypergeometric function. We return to consider $f(y)$ later. The results for the series in equation (9) are given in Table I. One can see that the estimate is remarkably good with the accuracy improving as N and M increase.

Next consider the series

$${}_2F_0\left(\frac{1}{4}, \frac{3}{4}; -x\right) = \sum_{n=1}^{\infty} (-1)^n \frac{(1/4)(3/4)\ldots(4n-1)/4}{n!} x^n \quad (11)$$

In spite of the fact that this is a diverging series, it can be seen from Table II that the estimates for the coefficients are excellent, improving as N and M increase. Note that the terms rapidly increase in magnitude.

We now turn to two examples from condensed matter theory. We first consider the two-dimensional square lattice and its magnetic susceptibility $\chi(w)$, where

$$w = \tanh(J/kT) \quad (12)$$

Table I. $[f(y)]^{-1}$, where $f(y) = {}_2F_0(1, 1, -y)$, Is the Euler Series[a]

$[N, M]$	No. of input coefficients	Padé	Exact	% error
[0, 1]	2	+1	−1	—
[0, 2]	3	−3	+3	—
[1, 1]	3	+1	+3	67
[1, 2]	4	−7	−13	46
[1, 3]	5	47	71	34
[2, 2]	5	59	71	17
[2, 3]	6	−413	−461	10
[2, 4]	7	3207	3447	7
[3, 3]	7	3303	3447	4.2
[3, 4]	8	−28,373	−29,093	2.5

[a]See Tables VII and VIII.

Table II. Values for the Series ${}_2F_0(\frac{1}{4}, \frac{3}{4}, -x)$ given in Equation (11)

$[N, M]$	No. of input coefficients	Padé	Exact	% error
[1, 1]	3	-0.22	-0.42	47
[2, 1]	4	0.872	1.289	32
[1, 2]	4	0.912	1.289	29
[3, 3]	7	-150.3	-157.8	4.7
[6, 5]	12	8.827×10^6	8.845×10^6	0.2
[5, 6]	12	8.827×10^6	8.845×10^6	0.2
[6, 6]	13	-1.0616×10^8	-1.0627×10^8	0.1
[8, 7]	16	2.9086×10^{11}	2.9090×10^{11}	0.015
[7, 8]	16	2.90859×10^{11}	2.9090×10^{11}	0.015
[9, 9]	19	-1.42686×10^{15}	-1.42689×10^{15}	0.002
[10, 9]	20	2.71240×10^{16}	2.71243×10^{16}	0.001
[9, 10]	20	2.71240×10^{16}	2.71243×10^{16}	0.001
[10, 10]	21	-5.42725×10^{17}	-5.42728×10^{17}	0.001
[10, 11]	22	1.140189×10^{19}	1.140192×10^{19}	0.003

This is the high-temperature expansion for the Ising model of ferromagnetism. The series is given by (Baker, 1975, p. 10)

$$\begin{aligned}\frac{d \ln \chi}{dw} = 4 &+ 8w + 28w^2 + 48w^3 + 164w^4 \\ &+ 296w^5 + 956w^6 + 1760w^7 + 5428w^8 \\ &+ 10{,}568w^9 + 31{,}068w^{10} + 62{,}640w^{11} \\ &+ 179{,}092w^{12} + 369{,}160w^{13} + 1{,}034{,}828w^{14} \end{aligned} \tag{13}$$

The results are shown in Table III. Again the estimates are excellent and the accuracy improves as N and M increase.

We next consider the high-temperature expansion of the magnetic susceptibility $\chi(x)$ for the spin-$\frac{1}{2}$ Heisenberg model. The expansion is given by (Baker, 1975, p. 276)

$$\begin{aligned}\chi(x) = 1 &+ 12x + 240x^2 + 6624x^3 \\ &+ 234{,}720x^4 + 10{,}208{,}832x^5 + 526{,}810{,}176x^6 \\ &+ 31{,}434{,}585{,}600x^7 + 2{,}127{,}785{,}025{,}024x^8 \\ &+ 161{,}064{,}469{,}168{,}128x^9 \qquad \text{where} \quad x = E/kT \end{aligned} \tag{14}$$

The results are shown in Table IV. Again the results are excellent and the accuracy improves as N and M increase. Moreover, we use the [4, 5] Padé to predict the next (unknown) term.

Table III. $(d \ln \chi)/dw$, Where χ is the Magnetic Susceptibility for the 2D Square Lattice Ising Model of Ferromagnetism (High-Temperature Expansion)

$[N, M]$	No. of input coefficients	Padé	Exact	% error
[1, 1]	3	98	48	104
[1, 2]	4	201	164	22.8
[2, 1]	4	82	164	49.8
[2, 2]	5	288	296	2.8
[2, 3]	6	961	956	0.48
[3, 2]	6	963	956	0.76
[3, 3]	7	1820	1760	3.4
[3, 4]	8	4876	5428	10.2
[4, 3]	8	5172	5428	4.7
[4, 4]	9	10,160	10,568	3.9
[4, 5]	10	33,584	31,068	8.1
[5, 4]	10	33,932	31,068	9.2
[5, 5]	11	67,746	62,640	8.2
[5, 6]	12	177,201	179,092	1.1
[6, 5]	12	178,461	179,092	0.35
[6, 6]	13	370,472	369,160	0.36
[6, 7]	14	1,033,105	1,034,828	0.17
[7, 6]	14	1,034,923	1,034,828	0.009
[7, 7]	15	2,172,702	NT	—

Table IV. High-Temperature Magnetic Susceptibility for a Spin-1/2 Heisenberg Model in a Three-space-dimensional Face-Centered Cubic Lattice

$[N, M]$	No. of input coefficients	Padé	Exact	% error
[0, 1]	2	144	240	40
[0, 2]	3	4032	6624	39
[1, 1]	3	4800	6624	28
[1, 2]	4	203,616	234,720	13
[1, 3]	5	9,230,112	10,208,832	10
[2, 2]	5	9,387,269	10,208,832	8
[2, 3]	6	5.0641×10^{8}	5.2681×10^{8}	4
[2, 4]	7	3.0639×10^{10}	3.1435×10^{10}	2.5
[3, 3]	7	3.0720×10^{10}	3.1435×10^{10}	2.3
[3, 4]	8	2.1045×10^{12}	2.1278×10^{12}	1.1
[3, 5]	9	1.5997×10^{14}	1.6106×10^{14}	0.7
[4, 4]	9	1.6005×10^{14}	1.6106×10^{14}	0.6
[4, 5]	10	1.3444×10^{16}	NT	—

Table V. Five-Loop Beta Function $g\phi^4$ Theory

$[N, M]$	No. of input coefficients	Padé	Exact	% error
[0, 1]	2	5.35	16.27	67
[0, 2]	3	−51.4	−135.8	62
[1, 1]	3	−93.4	−135.8	31
[2, 1]	4	1,133.5	1,424.3	20
[1, 2]	4	1,187.5	1,424.3	17
[1, 3]	5	−15,652	NT	—
[3, 1]	5	−14,938	NT	—
[2, 2]	5	−16,312	NT	—

We now turn to examples from PQFT in high-energy physics. Our first example is the five-loop beta function from $g\phi^4$ theory (Kleinert, 1991). The beta function $\beta(g)$ is given by

$$\beta(g) = 1.5g^2 - 2.83g^3 + 16.27g^4 - 135.8g^5 + 1424.3g^6 \tag{15}$$

The results are shown in Table V. Again the results are very good and the percent error decreases as one goes to higher order.

Let us now consider the three-loop QCD β function (Tarasov *et al.*, 1980) for various values of N_c, the number of colors, and N_f, the number of quark flavors. The results are shown in Table VI. The estimate is from equation I, the next term I (NT I) is also from equation I, and NT II is from equation II of equations (8). It can be seen that there is very good agreement over a large range of N_c and N_f. In fact, one can show that there is good agreement in the large-N_c ($\gg 1$) limit and this is a good approximation even for $N_c = 3$!

Next we turn to the Euler series which is Borel summable and which is asymptotic to

$$E(x) = \int_0^\infty \frac{e^{-t}}{1 + tx}\, dt \tag{16}$$

We will analyze the series

$$E(x) = \sum_{n=0}^{\infty} (-1)^n n!\, x^n \tag{17}$$

in some detail, as we believe PQFT series are also asymptotic series. (Although ϕ^4 theory is Borel summable, QCD is not. However, nonperturbative effects may render the Borel integral finite in QCD.)

West (1991) has also analyzed this series. The terms decrease until a minimum is reached and then increase without bound. For QED this occurs at order approximately $\alpha^{-1} \sim 137$ and we need not worry too much,

Table VI. QCD Beta Function for Various N_c and N_f[a]

N_c	N_f	Exact	Estimate	NT I	NT II
3	0	1429	946	20,006	17,722
	1	1155	772	14,930	13,292
	3	644	455	6477	5920
	5	181	195	846	841
4	0	3386	2242	63,229	56,010
	3	1956	1336	29,408	26,453
	6	672	583	5733	5631
5	0	6613	4379	154,367	136,743
	5	2940	2065	49,099	44,753
	8	981	958	8629	8624
6	0	11,428	7567	320,096	283,550
	6	5068	3556	101,502	92,472
	10	1321	1461	11,658	11,528
8	6	15,561	10,595	467,414	419,807
	9	10,244	7362	253,190	233,149
	13	3616	3694	47,329	47,307
10	6	34,694	23,380	1,377,319	1,230,853
	14	12,726	10,201	306,685	294,621
	16	7648	7500	132,437	132,388
14	6	109,035	72,914	6,399,395	5,697,112
	17	48,194	35,475	1,949,804	1,814,000
	23	17,965	19,028	389,956	388,592
18	29	42,709	42,700	1,292,209	1,292,208
22	36	71,208	74,522	2,467,455	2,462,110
26	40	160,586	145,072	8,170,562	8,094,304

[a]The last four columns are multiplied by -1.

but for QCD it may occur much earlier, since order α_s^{-1} may be much smaller.

The common belief, shared by West, is that one should stop when the minimum is reached and this gives the most accurate value possible. For $x = 0.1$, one should keep eight terms and one obtains three-figure agreement with the result obtained from (16),

$$E(0.1) = 0.91563333939788 \tag{18}$$

For $x = 0.2$, one should keep only four terms and one obtains only one-figure agreement with the result obtained from (16),

$$E(0.2) = 0.852110881422367 \tag{19}$$

This is true if one uses the partial sums, which can be seen from Tables VII and VIII. However if one uses the PA $[N, M]$ one can obtain 14-figure agreement with equations (13) and (14)! The prediction for the next term

Table VII. $\sum(-1)^n n!\, x^n$ for $x = 0.1^a$

[N, M]	Padé	Partial sum	Exact NT	Estimated NT
[1, 1]	0.9167	0.92	-6.0	-4.0
[1, 2]	0.9155	0.914	24.0	20.0
[2, 1]	0.9154	0.914	24.0	18.0
[5, 5]	0.91563334	0.9158	-3.99×10^7	-3.98×10^7
[5, 6]	0.915633338	0.9154	4.79×10^8	4.78×10^8
[6, 5]	0.915633337	0.9154	4.79×10^8	4.78×10^8
[10, 10]	0.915633339398	0.9319	-5.10909×10^{19}	-5.10908×10^{19}
[10, 11]	0.915633339398	0.88	1.1240007×10^{21}	1.123999×10^{21}
[11, 10]	0.915633339398	0.88	1.1240007×10^{21}	1.123999×10^{21}
[15, 15]	0.91563333939788	2×10^2	$-8.22283865 \times 10^{33}$	$-8.22283863 \times 10^{33}$
[15, 16]	0.91563333939788	-6×10^2	$2.631308369 \times 10^{35}$	$2.631308365 \times 10^{35}$
[16, 15]	0.91563333939788	-6×10^2	$2.631308369 \times 10^{35}$	$2.631308365 \times 10^{35}$

[a]The series is asymptotic to $E(0.1) = 0.91563333939788$.

Table VIII. $\sum(-1)^n n!\, x^n$ for $x = 0.2^a$

[N, M]	Padé	Partial sum	Exact NT	Estimated NT
[1, 1]	0.857	0.88	-6.0	-4.0
[1, 2]	0.851	0.83	24.0	20.0
[2, 1]	0.850	0.83	24.0	18.0
[5, 5]	0.8521116	1.1	-3.992×10^7	-3.983×10^7
[5, 6]	0.8521106	0.285	4.79×10^8	4.78×10^8
[6, 5]	0.8521105	0.285	4.79×10^8	4.78×10^8
[10, 10]	0.8521108818	2.05×10^4	-5.10909×10^{19}	-5.10908×10^{19}
[10, 11]	0.8521108812	-8.7×10^4	1.1240007×10^{21}	1.1239991×10^{21}
[11, 10]	0.8521108812	-8.7×10^4	1.1240007×10^{21}	1.1239990×10^{21}
[15, 15]	0.852110881425	2.4×10^{11}	$-8.22283865 \times 10^{33}$	$-8.22283863 \times 10^{33}$
[15, 16]	0.8521108814232	-1.52×10^{12}	$2.631308369 \times 10^{35}$	$2.631308365 \times 10^{35}$
[16, 15]	0.8521108814231	-1.52×10^{12}	$2.631308369 \times 10^{35}$	$2.631308365 \times 10^{35}$
[21, 21]	0.85211088142366	5.52×10^{21}	$-6.041526306337 \times 10^{52}$	$-6.041526306332 \times 10^{52}$
[21, 22]	0.85211088142366	-4.76×10^{22}	$2.658271574788 \times 10^{54}$	$2.658271574787 \times 10^{54}$
[22, 21]	0.85211088142366	-4.76×10^{22}	$2.658271574788 \times 10^{54}$	$2.658271574787 \times 10^{54}$

[a]The series is asymptotic to $E(0.2) = 0.85211088142366$.

(NT) is also excellent! In fact, we can push the accuracy even higher. The only limitation seems to be rounding problems which will eventually occur (we used quadra-precision). In fact, just for fun, I pushed the accuracy up and obtained, for $x = 0.1$, agreement with the integral in (16) to 33 significant figures! Thus, in perturbative QCD, where one is limited by the large value of α_s, especially at low energies, one may use PA and improve the possible accuracy considerably. Note in Tables VII and VIII that the exact next term (NT) and the estimated NT, although they agree, are both very large, for large M and N. Moreover, the partial sums oscillate wildly. However, the PA $[N, M]$ converges beautifully to $E(x)$!

In conclusion, we have estimated, from PAs, several examples from PQFT, from both condensed matter theory and high-energy physics. The results are excellent! Moreover, we have studied an asymptotic series and have shown that one can obtain extremely accurate results from the PAs, while the partial sums can give only two or three figures.

After this work was done, we received a preprint from J. Fleischer *et al.* (1990) in which PAs are used to estimate the perturbative coefficients for

$$R = \sigma_{tot}(e^+ e^- \to \text{hadrons})/\sigma(e^+ e^- \to \mu^+ \mu^-) \tag{20}$$

$\chi(x)$ [up to x^5, see equation (8)], $\beta(g)$ [see equation (9)], and the four loop β function of QCD (for $N_c = 3$ and $N_f = 5$), $\beta_3^{[1,1]}$. Unfortunately, they used incorrect values for R and $\beta(g)$. Our results for $\chi(x)$ (up to x^5) and $\beta_3^{[1,1]}$ agree.

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REFERENCES

Baker, G. A., Jr. (1975). *Essentials of Padé Approximants*, Academic Press, p. 10.

Fleischer, J., Pindor, M., Raczka, P. A., and Raczka, R. (1990). What may be expected from perturbative QCD in four-loop order and beyond, in *Proceedings of the XII Warsaw Symposium on Elementary Particle Physics, Kazimierz, Poland (May 29–June 2, 1989)*, Z. Ajduk, S. Pokorski, and A. K. Wroblewski, eds., World Scientific.

Kleinert, H., Neu, J., Schulte-Frohlinde, V., Chetyrkin, K. G., and Larin, S. A. (1991). *Physics Letters B*, **272**, 39.

Samuel, M. A., Li, G., and Steinfelds, E. (1992). PA and the R and R_τ ratios in PQCD, Fermilab Pub 92/200-T (July 1992).

Samuel, M. A., Li, G., and Steinfelds, E. (1993). *Physical Review D*, **48**, 869.

Samuel, M. A., Li, G., and Steinfelds, E. (1994). *Physics Letters B*, **323**, 188.

Tarasov, O. V., Vladimirov, A. A., and Zharkov, A. Yu. (1980). *Physics Letters*, **93B**, 429.

West, G. B. (1991). Why leading order QCD perturbation theory works so well even though the series is divergent and the coupling large, Los Alamos LA-UR-91, 3460.