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Estimating Perturbative Coefficients in Quantum Field Theory and the Ortho-Positronium Decay Rate Discrepancy*

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ABSTRACT

A method to estimate perturbative coefficients in High Energy Physics, Condensed Matter Theory and Statistical Physics is presented. It is shown to be accurate for a wide class of expansions. It is then applied to the ortho-positronium decay rate, where a discrepancy between theory and experiment has persisted for seven years. This difference is reduced to less than 2σ. In the case of para-positronium, the agreement between theory and experiment persists.

It has long been a hope in perturbative quantum field theory (PQFT), first expressed by Richard Feynman, to be able to estimate, in a given order, the result for the coefficient, without the brute force evaluation of all the Feynman diagrams contributing in this order. As one goes to higher and higher order the number of diagrams, and the complexity of each, increases very rapidly. Feynman suggested that even a way of determining the sign of the contribution would be useful.

The Standard Model (SM) of particle physics seems to work extremely well. This includes Quantum Chromodynamics (QCD), the Electroweak Theory as manifested in the Weinberg-Glashow-Salam Model and Quantum Electrodynamics (QED). In each case, however, we must use perturbation theory and compute large numbers of Feynman diagrams. In most of these calculations, however, we have no idea of the size or sign of the result until the computation is completed.

Recently we proposed [1] a method to estimate coefficients in a given order of PQFT, without actually evaluating all of the Feynman diagrams in this order. In this Letter we would like to present our method to a wider audience and demonstrate that it works for a large class of expansions in Quantum Field Theory, High Energy Physics, Condensed Matter Theory and Statistical Physics. In addition we will show that the long-standing discrepancy [2,3] between theory and experiment for the ortho-positronium decay rate is resolved, if one uses our estimate for the next coefficient in the expansion. The good agreement between theory and experiment in the case of para-positronium persists and we will obtain a new theoretical prediction which is 40 times more accurate than the current experimental value. We await a new more accurate experimental measurement for the para-positronium decay rate.

Our method makes use of Padé Approximants (PA) with which we can predict the next term S_{n+m+1} in the perturbation series S given by

$$S = S_0 + S_1 x + \cdots + S_{n+m} x^{n+m} \ . \tag{1}$$

We begin by defining the Padé approximant (type I)

$$[n,m] = \frac{a_0 + a_1 x + \cdots + a_n x^n}{1 + b_1 x + \cdots + b_m x^m} \tag{2}$$

to the series S where we set

$$[n,m] = S + O(x^{n+m+1}) \ . \tag{3}$$

We have written a computer program which solves Eq. (3) in general and then predicts the coefficient of the next term S_{n+m+1}. We call this estimate the Padé Approximant Prediction (PAP). Moreover we have derived algebraic formulae for the $[n,1]$, $[n,2]$, $[n,3]$ and $[n,4]$ PAP's. We present here only the $[n,1]$ and $[n,2]$ PAP's since the $[n,3]$ and $[n,4]$ are too complicated to be presented here and will be included in the long, detailed paper to follow [4].

Our results for the $[n,1]$ and $[n,2]$ PAP's are:

$$S_{n+2} = \frac{S_{n+1}^2}{S_n} \qquad [n,1] \tag{4}$$

$$S_{n+3} = \frac{2S_n S_{n+1} S_{n+2} - S_{n-1} S_{n+2}^2 - S_{n+1}^3}{S_n^2 - S_{n-1} S_{n+1}} \qquad [n,2] \ . \tag{5}$$

As indicated above one can step up or down in n for m fixed in the $[n,m]$ PAP. When stepping down one should put $S_{-1} = 0$.

We have shown [1,5] that our method works for a large number of cases in PQFT, Condensed Matter Theory and Statistical Physics. These include the anomalous magnetic moment of the muon, the tau lepton, and the electron, which we will reconsider here, the R_τ ratio and the β function in Perturbative Quantum Chromodynamics (PQCD), various Sum Rules in PQCD, the 5 loop β function in $g\phi^4$ theory, high-temperature expansions for the magnetic susceptibility in Condensed Matter Theory, a large number of expansions in Statistical Physics and many mathematical examples.

We begin with the R_τ ratio [6] in the MS and $\overline{\mathrm{MS}}$ schemes. R_τ is defined by

$$R_\tau = \frac{\Gamma(\tau \to v + \text{hadrons})}{\Gamma(\tau \to e v \overline{v})} . \tag{6}$$

The results are shown in Tables I and II respectively for various numbers of fermions N_f. Also shown are two predictions for the next-unknown term S_4. It can be seen that the estimates are excellent and the [1,2] and the [2,1] PAP's for S_4 agree very well with each other. Next we present the result for

$$R = \frac{\sigma_{tot}(e^+e^- \to \text{hadrons})}{\sigma(e^+e^- \to \mu^+\mu^-)} . \tag{7}$$

The results in the MS and $\overline{\mathrm{MS}}$ [6,7] are shown in Tables III and IV respectively. The results in the MS scheme are very good, however, the results in the $\overline{\mathrm{MS}}$ scheme are not too good. The sign of S_3 cannot be predicted correctly since the sign pattern is (+++−). In such cases one needs more terms for the PAP to be accurate.

We next consider

$$a_e \equiv \frac{g-2}{2} \tag{8}$$

for the electron [8]. Our results are shown in Tables V and VI. It can be seen in Table V that the estimates are pretty good, especially the [0,2] PAP. In Table VI we give our prediction for the next-unknown term (NT) and the next-next-unknown term (NNT).

In Tables VII and VIII we present two representative examples from Condensed Matter Theory [9]. It can be seen that the PAP's are excellent! Moreover the percent error decreases as n and m increase!

In Tables IX and X we give two representative examples from Statistical Physics. In both cases the PAP is excellent and the error decreases as n and m increase! The number in parenthesis refers to the power of 10, *e.g.* $0.83(-10) = 0.83 \times 10^{-10}$. We will present more examples from Condensed Matter Theory and Statistical Physics in our long paper.

Finally we come to the positronium decay rates. For ortho-positronium there has been a discrepancy between theory and experiment for seven years! The decay rate is given by

$$\lambda_{th} = \lambda_0 \left\{ 1 + A\left(\frac{\alpha}{\pi}\right) + \frac{1}{3}\alpha^2 \ell n\, \alpha + B\left(\frac{\alpha}{\pi}\right)^2 + N\left(\frac{\alpha}{\pi}\right)^3 + M\alpha^3 \ell n^2 \alpha \right\} \qquad (9)$$

where

$$\lambda_0 = \frac{\alpha^6 mc^2 2(\pi^2 - 9)}{\hbar\, 9\pi} \,. \qquad (10)$$

The current situation is given by:

$$\begin{aligned} A &= -10.282(3) \\ B &= N = M = 0 \\ \lambda_{th}^{(1)} &= 7.03831(7)\, \mu s^{-1} \,. \end{aligned} \qquad (11)$$

The most recent experimental result [3] is

$$\lambda_{ex} = 7.0482(16)\, \mu s^{-1} \,. \qquad (12)$$

In this experiment positronium was formed in a vacuum. This yields a difference

$$\lambda_{ex} - \lambda_{th}^{(1)} = 0.0099(16) \ , \tag{13}$$

a 6.2σ discrepancy between theory and experiment. The previous experiment was a gas experiment in which positronium was formed in Isobutane, Neopentane, N_2 and Ne. That result [2] was

$$\lambda_{ex} = 7.0516(13)\,\mu s^{-1} \tag{14}$$

and led to a difference

$$\lambda_{ex} - \lambda_{th}^{(1)} = 0.0133(13)\,\mu s^{-1} \ , \tag{15}$$

a 10σ discrepancy! However it was later suggested that the extrapolation to zero pressure was understood only for N_2 and Ne for which the result was [3]

$$\lambda_{ex} = 7.0492(15)\,\mu s^{-1} \tag{16}$$

in good agreement with the vacuum experimental result in Eq. (12). We will therefore use the result in Eq. (12) in the following analysis.

The PAP [0,1] for B is

$$B = 105.7 \tag{17}$$

which leads to a theoretical prediction

$$\lambda_{th}^{(2)} = 7.04243\,\mu s^{-1} \tag{18}$$

and

$$\lambda_{ex} - \lambda_{th}^{(2)} = 0.0058(16)\,\mu s^{-1} \ , \tag{19}$$

only a 3.6σ difference. Moreover $\lambda_{th}^{(2)}$ should have an estimated error associated with it. We estimate $|M| < 25$ and $|N| < 10,000$ and hence

$$\lambda_{th}^{(2)} = 7.0424(26)\,\mu s^{-1} \tag{20}$$

and $\lambda_{ex} - \lambda_{th}^{(2)} = 0.0058(31)\,\mu s^{-1}$, only a 1.9σ difference! Alternatively we could estimate an error for B and obtain

$$B = 106(67) = 106 \pm 67 \ . \tag{21}$$

Thus the original 10σ discrepancy in Eq. (15) has now been reduced to a difference of less than 2σ and, hence, the ortho-positronium decay rate discrepancy has been resolved!

In the case of para-positronium [10,11] there is agreement between theory and experiment and we should make sure that this agreement is not spoiled by the PAP. The decay rate for para-positronium is

$$\lambda_{th} = \lambda_0 \left\{ 1 + A\left(\frac{\alpha}{\pi}\right) - 2\alpha^2 \ell n \alpha + B\left(\frac{\alpha}{\pi}\right)^2 + N\left(\frac{\alpha}{\pi}\right)^3 + M\alpha^3 \ell n^2 \alpha \right\} \tag{22}$$

where $\lambda_0 = \alpha^5 mc^2/2\hbar$ and

$$A = \frac{\pi^2}{4} - 5 \tag{23}$$

with $B = N = M = 0$,

$$\lambda_{th}^{(1)} = 7.989460(1)\,ns^{-1} \ . \tag{24}$$

The experimental value [11] is

$$\lambda_{ex} = 7.994(11)\,ns^{-1} \tag{25}$$

and

$$\lambda_{ex} - \lambda_{th}^{(1)} = 0.0045(110)\, ns^{-1} \ . \tag{26}$$

This difference is only 0.41σ!

The PAP [0,1] is

$$B = 6.4141 \tag{27}$$

which leads to

$$\lambda_{th}^{(2)} = 7.98974\, ns^{-1} \tag{28}$$

and

$$\lambda_{ex} - \lambda_{th}^{(2)} = 0.0043(110) \ , \tag{29}$$

a 0.39σ difference. Now we should estimate the error in $\lambda_{th}^{(2)}$. We use $|M| < 25$ and $|N| < 1000$, which leads to

$$\lambda_{th}^{(2)} = 7.98974(25)\, ns^{-1} \tag{30}$$

and $\lambda_{ex} - \lambda_{th}^{(2)}$ is unchanged from the result given in Eq. (29). It should be noted that the present experimental error is 44 times the theoretical error given in Eq. (30). Hence we eagerly await more precise experiments to measure the para-positronium decay rate.

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TABLE I

R_τ in the MS Scheme

N_f	ESTIMATE [1,1] S_3	EXACT S_3	[1,2] S_4	[2,1] S_4
0	137	158	2135	2132
1	121	137	1717	1715
2	106	118	1349	1347
3	92.1	99.2	1026	1025
4	79.0	81.7	751	750
5	67.0	65.2	518	518
6	56.0	49.7	330	330

TABLE II

R_τ in the $\overline{\rm MS}$ Scheme

N_f	ESTIMATE [1,1] S_3	EXACT S_3	[1,2] S_4	[2,1] S_4
0	40.3	48.6	376	372
1	35.5	40.9	281	280
2	31.1	33.5	201	201
3	27.1	26.4	134	134
4	23.3	19.6	80.3	79.6
5	19.8	13.1	41.7	38.8
6	16.5	7.0	19.3	12.0

TABLE III

R in the MS Scheme

N_f	ESTIMATE [1,1] S_3	EXACT S_3	[1,2] S_4	[2,1] S_4
0	54.2	56.0	426.6	426.5
1	47.9	47.4	325.1	325.1
2	42.0	39.2	237.1	236.9
3	36.4	31.3	162.9	162.0
4	31.3	23.7	102.8	100.6
5	26.6	16.5	57.7	53.0
6	22.2	9.7	28.9	19.9

TABLE IV

R in the $\overline{\mathrm{MS}}$ Scheme

N_f	ESTIMATE [1,1] S_3	EXACT S_3	[1,2] S_4	[2,1] S_4
0	3.9	–6.6	79.4	22.2
1	3.5	–7.8	111.8	32.9
2	3.1	–9.1	157.9	46.7
3	2.7	–10.3	224	64.4
4	2.3	–11.5	326	87.0
5	2.0	–12.8	491	116
6	1.7	–14.0	794	152

TABLE V

$$a_e = x/2 - 0.3285\,x^2 + 1.1765\,x^3 - 1.43\,x^4$$

$x = \alpha/\pi$	ESTIMATE	EXACT
[0,1]	0.22	1.1765
[1,1]	−4.21	−1.43
[2,1]	1.74	NT
[3,1]	$-2.12(S_4 = 1.74)$	NNT
[3,1]	$-7.25(S_4 = 3.22)$	NNT
[0,2]	−1.40	−1.43
[1,2]	3.22	NT
[2,2]	$-2.12(S_4 = 1.74)$	NNT
[2,2]	$-4.93(S_4 = 3.22)$	NNT
[1,3]	$-4.93(S_4 = 3.22)$	NNT

TABLE VI

a_e: Predictions for the next-term and the next-next term.

NT	[2,1]	1.74
	[1,2]	3.22
	[0,1]	2.77 (+)
	AVERAGE	2.6(8)
NNT	[3,1]	$-2.12(S_4 = 1.74)$
	[3,1]	$-7.25(S_4 = 3.22)$
	[2,2]	$-2.12(S_4 = 1.74)$
	[2,2]	$-4.93(S_4 = 3.22)$
	[0,1]	$-6.23(-)$
	[1,3]	$-4.93(S_4 = 3.22)$
	AVERAGE	$-4.6(2.7)$

TABLE VII

$d\ell n\,\chi/dw$ where χ is the magnetic susceptibility for the 2-D square lattice Ising Model of Ferromagnetism (high temperature expansion).

$[n,m]$	Number 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	N.T.	—

TABLE VIII

High Temperature Magnetic Susceptibility for a spin-1/2 Heisenberg Model in a 3-space dimensional face-centered cubic lattice

$[n, m]$	Number 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}	N.T.	—

TABLE IX

High Temperature Susceptibility Series of the Square-Lattice Ising Model

$[n,m]$	Padé	Exact	% Error
[0,1]	16	12	33
[1,2]	108	100	8
[3,3]	1972	1972	0
[3,4]	5188	5172	0.31
[4,3]	5188	5172	0.31
[5,4]	34856	34876	0.057
[5,5]	89764	89764	0
[5,6]	229704	229628	0.033
[7,6]	1486858	1486308	0.037
[7,7]	3764311	3763460	0.023
[8.7]	9496081	9497380	0.014
[12,12]	36212337725	36212402548	0.18(−3)
[12,13]	89896881041	89896870204	0.12(−4)
[20,20]	68849212197681(3)	68849212197172(3)	0.74(−9)
[20,21]	169150097346(6)	169150097365(6)	0.11(−7)
[21,21]	41541963877(7)	41541963949(7)	0.17(−6)
[21,22]	1019816266329(6)	1019816266253(6)	0.75(−8)
[24,23]	36912183773288(6)	36912183772985(6)	0.82(−9)
[24,24]	90466431959184(6)	90466431959612(6)	0.47(−9)
[24,25]	22164947092629(7)	22164947092555(7)	0.33(−9)
[25,24]	221649470925546(6)	22164947092555(6)	0.38(−11)
[26,25]	13294400774266(8)	13294400774247(8)	0.14(−9)
[26,26]	32546159798889(8)	32546159798489(8)	0.12(−8)
[27,26]	79654880661744(8)	79654880659405(8)	0.29(−8)
[26,27]	79654880659339(8)	79654880659405(8)	0.83(−10)
[27,27]	194906447358589(8)	N.T.	—

TABLE X

Number of closed Polygons on a Square Lattice

$[n, m]$	Padé	Exact	% Error
[0,1]	4	7	43
[1,1]	24.5	28	13
[1,2]	114.3	124	7.8
[3,3]	15641.4	15268	2.4
[3,4]	81603.2	81826	0.27
[5,4]	2520776.4	2521270	0.02
[5,5]	14382759.9	14385376	0.018
[5,6]	83301403.3	83290424	0.013
[7,7]	17332403704.6	17332874364	0.27(−2)
[7,8]	104653043328.9	104653427012	0.37(−3)
[8,8]	636737111378.9	636737003384	0.17(−4)
[8,9]	3900768657365.8	3900770002646	0.34(−4)
[9,8]	3900768645591.6	3900770002646	0.35(−4)
[9,9]	24045477087166.3	24045500114388	0.96(−4)
[9,10]	149059818372329	149059814328236	0.27(−5)
[10,9]	149059814952508	149059814328236	0.42(−6)
[10,10]	928782402852355	928782423033008	0.22(−5)
[10,11]	5814401458255866	5814401613289290	0.27(−5)
[11,10]	5814400906586723	5814401613289290	0.12(−4)
[11,11]	36556766563181916	36556766640745936	0.21(−6)
[11,12]	230757492329413778	230757492737449632	0.18(−6)
[12,11]	230757492299121126	230757492737449632	0.19(−6)
[12,12]	1461972664107671386	1461972662850874880	0.86(−7)
[12,13]	9293993426515280515	9293993428791900928	0.24(−7)
[13,12]	9293993426247752549	9293993428791900928	0.27(−7)
[13,13]	592709055867(8)	N.T.	—