Resummation of perturbative QCD by Padé approximants

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Abstract
In this lecture I present some of the new developments concerning the use of Padé Approximants (PA’s) for resumming perturbative series in QCD. It is shown that PA’s tend to reduce the renormalization scale and scheme dependence as compared to truncated series. In particular it is proven that in the limit where the $\beta$ function is dominated by the 1-loop contribution, there is an exact symmetry that guarantees invariance of diagonal PA’s under changing the renormalization scale. In addition it is shown that in the large $\beta_0$ approximation diagonal PA’s can be interpreted as a systematic method for approximating the flow of momentum in Feynman diagrams. This corresponds to a new multiple scale generalization of the Brodsky-Lepage-Mackenzie (BLM) method to higher orders. I illustrate the method with the Bjorken sum rule and the vacuum polarization function.

\footnote{1 A lecture given at the Cracow School of Theoretical Physics, Zakopane, May 30 – June 10, 1997}
I will talk about resummation of perturbative series in QCD. The basic question I deal with is how to use finite order perturbative calculations in QCD to make unambiguous theoretical predictions, with controlled errors. As experiments improve one requires the theoretical predictions to be more accurate. However, in QCD it is very hard to get accurate predictions, basically because the coupling constant is large. This leads to non-negligible non-perturbative effects as well as a badly divergent and renormalization scheme dependent perturbative series.

In this talk I will show that PA’s which start out as an alternative to a finite order perturbative series having the same formal accuracy, actually have an important advantage over the finite order series. Through the resummation of certain all-order effects related to the running of the coupling-constant, PA’s become independent of the choice of the renormalization scale and therefore lead to more accurate and more reliable predictions. The material presented in this lecture appears in greater detail in ref. [3, 4, 5].

The outline of the talk is as follows: I will start by introducing the PA’s method and the problem of renormalization scale dependence in QCD. I will mention some of the other ideas that were raised to confront the problem of renormalization scale dependence and show how PA’s solve it in a most elegant way. Then I will address the question of what higher order effects are summed-up by PA. I will show that there is a direct interpretation of PA’s in terms of approximating the momentum distribution of virtual gluons in Feynman diagrams.

First, what are PA and how do I use them? I start with an effective charge related to some physical observable, written as a power series in $x$:

$$S_n = x \left( 1 + r_1 x + r_2 x^2 + \cdots + r_n x^n \right)$$

(1)

where $x = \alpha_s / \pi$. A PA is constructed by writing a ratio of two polynomials such that when expanded back to a Taylor series, it gives the known coefficients $r_1$ through $r_n$:

$$P_{x[N/M]} = \frac{x \left( 1 + a_1 x + \cdots + a_N x^N \right)}{1 + b_1 x + \cdots + b_M x^M}$$

$$N + M = n$$

For a recent review on the nature of perturbative series and resummation techniques see ref. [1].

PA have various successful application in physics. Examples of applications to statistical physics and quantum field theory are listed in ref. [2]. Applications to QCD appear in ref. [3].
There is a theorem that for any degree $N$ in the numerator and $M$ in the denominator such that $N + M = n$ there is a unique PA function \[.\] I will mainly deal here with diagonal PA’s which are written, in my notation, as $x[N/N + 1]$, having one power of $x$ out of the brackets. I will soon come back to discuss PA’s.

A renormalized perturbative series in QCD is not expected to give exact predictions for measurable quantities due a few limitations. First, the series is divergent and not even Borel-summable. The resulting ambiguity is related to the existence of non-perturbative effects. Second, at any given order, the partial-sum depends on non-physical parameters, such as the renormalization scale. This also makes the prediction ambiguous.

Let us concentrate on the renormalization scale dependence. Usually, when we calculate some observable $R$ that depends on one external momentum $Q^2$ in perturbation theory, we choose as an expansion parameter the renormalized coupling-constant at the external scale $Q^2$. This “natural” choice of $\mu^2 = Q^2$ is, however, quite arbitrary. We can, just as well, use some other expansion parameter $y = \alpha_s(e^t Q^2)/\pi$, where $t \neq 0$. The renormalization group equation

$$\frac{dx}{dt} = \beta_0 x^2 + \beta_1 x^3 + \beta_2 x^4 + \cdots$$

determines how the two couplants are related,

$$x = y + \beta_0 t y^2 + \left(\beta_0^2 t^2 + \beta_1 t\right) y^3 + \left(\beta_0^3 t^3 + \frac{5}{2} \beta_1^2 t^2 + \beta_2 t\right) y^4 + \cdots$$

(2)

and thus how the finite order series can be written in terms of $y$:

$$\tilde{S}_n(t) = y \left(1 + \tilde{r}_1 y + \tilde{r}_2 y^2 + \tilde{r}_3 y^3 + \cdots + \tilde{r}_n y^n\right).$$

(3)

The new coefficients $\tilde{r}_i$ are different from the original coefficients $r_i$, so as to compensate for the scale shift, such that the total effect is some residual dependence on $t$ which is of the next, uncalculated order. Still, in QCD, since the coupling constant is large, the numerical difference due to the change of scale can be quite large. This limits the predictive power of the theory. Beyond two-loops, there is also the question of scheme dependence which can be parameterized by the higher-order coefficients of the $\beta$ function, $\beta_2$, $\beta_3$ and onward.
In order to test the significance of this scale and scheme dependence, we studied the polarized Bjorken Sum-Rule. In fig. 1 the Bjorken effective charge at NNLO for $Q^2 = 20\, GeV^2$ is plotted as a function of the renormalization group non-physical parameters: the coupling $x = \alpha_s(\mu^2)/\pi$ and the second coefficient of the $\beta$ function: $C_2 = \beta_2/\beta_0$. We see that the surface is far from being flat.

The same surface is drawn again in fig. 2, but here – as a contour plot. The thick lines are contours of equal effective charge. Large renormalization scheme dependence corresponds to large higher-order corrections, since these are required to compensate for the scale dependence. This observation makes it clear that we should carefully choose the renormalization scale and scheme that we are using. In fig. 2 one can identify a region of relatively low renormalization scale and scheme dependence. Specific scales and schemes are chosen according to different criterions such as the method of Effective Charges, the Principal of Minimal Sensitivity and the BLM scale-setting method. For the Bjorken Sum-Rule example (fig. 2), all of the above are located in the central region of low renormalization scale and scheme dependence. Note that in this case, $\overline{\text{MS}}$, with $\mu^2 = Q^2$ is not a good choice.

Let’s go back to eq. (2) that describes the scale transformation relating the coupling-constants $x$ and $y$ defined at two different scales. If we assume that the 1-loop coefficient of the $\beta$ function, $\beta_0$, is large enough, i.e.

$$\beta_0 \gg \beta_i x^i$$

for any $i \geq 1$, we can approximate the full relation by one that includes only the leading terms in $\beta_0$:

$$x \simeq y + \beta_0 t y^2 + \beta_0^2 t^2 y^3 + \beta_0^3 t^3 y^4 + \cdots$$

This can be written in a closed form:

$$x = \frac{y}{1 - \beta_0 ty}.$$ 

It is important to realize that in the physical case of QCD with 3 to 5 flavors, this approximation is good. Fig. 3 shows the renormalization scale transformation itself, namely the running coupling constant as a function of the scale. The dashed line is the best we know of the running coupling in
QCD (it includes the 4-loop effects), and the solid line is the 1-loop running coupling. The two are quite close and I shall use here the 1-loop formula.

I now get to the main point, which is the independence of PA on the renormalization scale. We saw that partial-sums as usually written in perturbation theory always yield different results in different renormalization scales:

\[ S_n(0) \neq \tilde{S}_n(t) \]

where \( S_n(0) \) refers to \( \mu^2 = Q^2 \) as in eq. (1), \( \tilde{S}_n(t) \) refers to \( \mu^2 = e^t Q^2 \) as in eq. (3), and \( x = y / (1 - \beta_0 ty) \). However, if we construct a diagonal PA from the series in \( x \) (eq. (1)),

\[
P_x[N/N+1](x) = x \frac{1 + a_1 x + \ldots + a_N x^N}{1 + b_1 x + \ldots + b_{N+1} x^{N+1}}
\]

and independently, another PA from the series in \( y \) (eq. (3)),

\[
\tilde{P}_y[N/N+1](y) = y \frac{1 + \tilde{a}_1 y + \ldots + \tilde{a}_N y^N}{1 + \tilde{b}_1 y + \ldots + \tilde{b}_{N+1} y^{N+1}}
\]

we will get the same result in both:

\[
P_x[N/N+1](x) = \tilde{P}_y[N/N+1](y).
\]

This is due to the mathematical property of diagonal PA’s: they are invariant under homographic transformations of the PA argument \( (x \to x/(1 + K x)) \), see [4, 6]. We know that the all-order result does not depend on the renormalization scale. The fact that diagonal PA are invariant suggests that they correctly resum certain all-order effects that are related to the running of the coupling-constant.

Non-diagonal PA are not exactly invariant. However, on the global level (for large scale shifts \( t \)) they always have a reduced scale dependence [4]. Going back to the example we examined above, namely the NNLO Bjorken sum-rule, we show in fig. 4 the \( x[0/2] \) PA. Clearly (compare with the partial-sum of fig. 1) the renormalization scale and scheme dependence is almost completely eliminated!

Non-diagonal PA’s may be dangerous, since specific renormalization scales and schemes are sometimes particularly deviant, as in the example of the
$x[1/1]$ PA for the Bjorken sum-rule shown in fig. 5. Therefore it is best to use a diagonal $x[N − 1/N]$ PA.

I now consider the question of what higher-order contributions are summed-up by diagonal PA’s. It turns out that we can get some rigorous results \cite{5} if we limit ourselves to the “large $\beta_0$” approximation \cite{10,11,12}, where only the leading term in $\beta_0$ in each perturbative coefficient is taken into account. This approximation corresponds to summing certain higher-order contributions that are related to the exchange of one virtual gluon. I use Neubert’s formulation \cite{10}, where resummation is achieved by using the running coupling-constant at the vertices. The resummation integral is then a weighted average of the coupling-constant at all scales:

$$A_{res} = \int w(k)\alpha_s(k^2)d^4k = \int_{-\infty}^{\infty} \rho(s)x^V(e^sQ^2)ds$$

where $w(k)$ is the Feynman integrand and $s = \ln\left(\frac{k^2}{Q^2}\right)$. The superscript $V$ stands for the V-scheme which is the most convenient renormalization scheme for my purposes. While a specific scheme is used here in order to simplify the formulae, it is important to understand that the above resummation integral is scheme-invariant \cite{10}. The function $\rho(s)$ describes the distribution of momentum of the exchanged gluon, and $x^V(e^sQ^2)$ describes the interaction strength as a function of the momentum. Using a 1-loop formula for $x^V(e^sQ^2)$ I get:

$$A_{res} = \int_{-\infty}^{\infty} \rho(s) \left( \frac{x^V(Q^2)}{1 + s\beta_0 x^V(Q^2)} \right) ds$$

Clearly the integral includes contributions from an infinite set of diagrams. The exact distribution function (in the large $\beta_0$ approximation) has been calculated for a few observables, such as the vacuum-polarization D-function \cite{13,14,10} which I shall use here as an example. A representative diagram is the following:
In this particular diagram the exchanged gluon is dressed by fermion loops. However, gluonic corrections that are related to the 1-loop running of the coupling are resummed in the above technique just as well.

Of course, the resummation integral is not well defined, due to the integration over the infra red pole in the 1-loop formula for the running coupling (Landau pole). This is how infra red renormalons appear in this formulation. I will not deal here with the renormalon ambiguity which cannot be settled completely within perturbative QCD, but rather use the resummation integral to study the PA method. The general methodology is to assume that only a first few coefficients in the perturbative series are known, construct a PA basing on this limited information and then compare the PA with the exact all-order result. We will see below that this comparison can be done also on the level of the momentum distribution function, since PA’s can be interpreted as what one obtains by replacing the continuous momentum distribution function with a particular discrete distribution.

It was found empirically that the momentum distribution function in the large $\beta_0$ approximation is a non-negative function in many physical examples [10, 5]. This justifies a posteriori the probabilistic interpretation implied by the name ‘momentum distribution’. If indeed $\rho(s) \geq 0$ for any $s$, then the resummation integral defines a so-called Hamburger function [3]:

$$f(z) \equiv A_{\text{res}}/\beta_0 = \int_{-\infty}^{\infty} \rho(s) \frac{z}{1 + sz} ds = \int_{-\infty}^{\infty} \frac{z}{1 + sz} d\phi(s).$$

(4)

where $z = \beta_0 x^V(Q^2)$ and $\phi(s)$ is the indefinite integral of $\rho(s)$. The pertur-
bative coefficients are moments of the distribution function:

\[ f_i = \int_{-\infty}^{\infty} s^i d\phi(s) \]

for \( i \geq 0 \).

There is a theorem \([6]\) that guarantees that for a Hamburger function, a \( z[N - 1/N] \) PA constructed from the partial-sum:

\[ z \sum_{i=0}^{2N-1} f_i(-z)^i \]

can be written as:

\[ f(z) \sim z[N - 1/N] = \sum_{i=1}^{N} \frac{r_i z}{1 + q_i z} \]

with \( q_i \) real and \( r_i > 0 \) for \( i = 1, 2, \ldots, N \).

Through this decomposition of the PA function, together with eq. (4) one realizes that the PA corresponds to approximating the all-order continuous distribution function by a sum of \( N \) weighted \( \delta \)-functions:

\[ \rho_N(s) = \sum_{i=1}^{N} r_i \delta(s - q_i) \]

or, equivalently, its indefinite integral \( \phi(s) \), by a piece-wise constant function composed of \( N \) steps:

\[ \phi_N(s) = \sum_{i=1}^{N} r_i \theta(s - q_i). \]

Note that \( \rho_N(s) \) is optimal (and unique, of course) since the equation for constructing the PA imply that \( \rho_N(s) \) reproduces the first \( 2N \) moments of the distribution function, which we know. Using a diagonal PA of a Hamburger function to identify the optimal scales \( (q_i) \) and weights \( (r_i) \) is the basic idea behind the method of Gaussian quadrature for numerical integration \([3]\).

In the Brodsky-Lepage-Mackenzie (BLM) approach \([9]\) one evaluates the coupling-constant at a scale that corresponds to the average momentum of the exchanged gluon (the BLM scale). This is exactly equivalent to approximating the distribution function by a single \( \delta \)-function located at its center.
This same effect can also be achieved simply by using a $x[0/1]$ PA for the leading $\beta_0$ series $[4]$. In the method described above one uses an $x[N-1/N]$ PA of the leading $\beta_0$ series that corresponds to approximating the momentum distribution function by a set of $N$ weighted $\delta$ functions. Therefore it can be viewed as a generalization of the BLM method for higher-orders.

In the following, I illustrate the above ideas with the vacuum-polarization D-function. The all-order distribution function $\rho(s) [10]$ is plotted in fig. 6 as a continuous line. We see that there are contributions from both UV scales (positive $s$) and IR scales (negative $s$). The different symbols correspond to the locations ($q_i$) and weights ($r_i$) of the diagonal PA’s poles. For the $x[0/1]$ PA, there is one $\delta$-function at the BLM scale. For the $x[1/2]$ PA, there are two $\delta$-functions, and so on. In Fig. 7 we see how using $x[N-1/N]$ PA corresponds to approximating the integral distribution function $\phi(s)$ by a piecewise constant function, composed of $N$ steps.

To conclude, we saw that diagonal PA’s can be used to resum certain all-order effects that are related to the running of the coupling constant, and thus provide a systematic method for obtaining reliable scale-invariant predictions. There is a rigorous relation between diagonal PA and the momentum distribution of virtual gluons. I stress that this result holds only for a single gluon exchange, i.e. within the large $\beta_0$ approximation. The way to go beyond this approximation is still unclear. Nevertheless, from the results presented here for the Bjorken Sum-Rule, it is clear that PA’s are an important tool for QCD phenomenology.

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Fig. 1

Bjorken effective-charge - a NNLO partial-sum
Bjorken effective-charge - a third order partial-sum
Fig. 3

Scale Transformation for $N_r=3$ vs. large $\beta_0$ approximation

Only $\beta_0$ terms
Including $\beta_1$, $\beta_2$, $\beta_3$

$(\tau)^x$
Bjorken effective-charge - [0/2] PS

Fig. 4
Bjorken effective-charge - [1/1] PS
Fig. 6

Momentum Distribution within the Adler D-function in the large $\beta_0$ limit vs. Padé-approximants $\delta$-function location.

$\langle s \rangle_d$
Fig. 7