Why Padé Approximants reduce the Renormalization-Scale dependence in QFT?

Einan Gardi

School of Physics and Astronomy
Raymond and Beverly Sackler Faculty of Exact Sciences
Tel-Aviv University, 69978 Tel-Aviv, Israel
e-mail: gardi@post.tau.ac.il

Abstract

We prove that in the limit where the $\beta$ function is dominated by the 1-loop contribution ("large $\beta_0$ limit") diagonal Padé Approximants (PA’s) of perturbative series become exactly renormalization scale (RS) independent. This symmetry suggest that diagonal PA’s are resumming correctly contributions from higher order diagrams that are responsible for the renormalization of the coupling-constant. Non-diagonal PA’s are not exactly invariant, but generally reduce the RS dependence as compared to partial-sums. In physical cases, higher-order corrections in the $\beta$ function break the symmetry softly, introducing a small scale and scheme dependence. We also compare the Padé resummation with the BLM method. We find that in the large-$N_f$ limit using the BLM scale is identical to resumming the series by a $x[0/n]$ non-diagonal PA.
1 Introduction

Padé Approximants (PA’s) have proven to be useful in many physics applications, including condensed-matter problems and quantum field theory [1]. We denote Padé Approximants (PA’s) to a perturbative QCD series, describing a generic effective-charge \( S(x) = x(1 + r_1 x + r_2 x^2 + \cdots + r_n x^n) \) by

\[
x[N/M] = x \frac{1 + a_1 x + \cdots + a_N x^N}{1 + b_1 x + \cdots + b_M x^M} : x[N/M] = S + x \mathcal{O}(x^{N+M+1})
\]

i.e. the PA’s are constructed so that their Taylor expansion up to and including order \( N+M = n \) is identical to the original series [1]. PA’s may be used either to predict the next term in some perturbative series, called a Padé Approximant prediction (PAP), or to estimate the sum of the entire series, called Padé Summation. The reasons for the success of PA’s in these different applications have not always been apparent. Indeed, rational functions are very flexible, and hence they are good candidates to approximate other unknown functions, but this does not seem as a sufficient explanation. In this paper we give for the first time an argument, based on renormalization group analysis, why PA’s are especially well suited for summation of series describing to observables in QFT.

Among the areas in which PA’s have had remarkable successes has been perturbative QCD [2,3] where PA’s applied to low-order perturbative series have been shown to ‘postdict’ accurately known higher-order terms, and also used to make estimates of even higher-order unknown terms that agree with independent predictions [4] based on the Principle of Minimal Sensitivity (PMS) [5] and Effective Charge (ECH) [6] techniques.

In recent papers [3,4] we used the Bjorken sum rule for deep-inelastic scattering of polarized electrons on polarized nucleons as a testing ground and showcase for the use of PA’s. We showed that applying the appropriate PA to the Bjorken Sum Rule, the renormalization scale (RS) and scheme dependence are significantly reduced. This observation provided circumstantial evidence that PA are resumming correctly the most important part of higher-order perturbative corrections. However, in absence of an explicit mathematical argument, we could not show that this success was not coincidental.

In this paper we provide the missing mathematical argument and prove that in the large \( \beta_0 \) limit (cf. Eq. (3) and (8)) when only 1-loop renormalization of the coupling is important (e.g. large-\( N_f \) QCD) diagonal PA are exactly RS invariant, giving the same result, regardless of the RS. This results directly from the fact that in the large \( \beta_0 \) limit the RS transformation of the coupling reduces to a homographic transformation of the Padé argument. Diagonal PA’s are invariant under

*We use this notation, with one power of \( x \) out of the brackets so that \( S(x) \) would fit the usual notation of effective charge. Note that the diagonal case in this notation is \( x[N/N + 1] \).
such transformations. Non-diagonal PA’s are not totally invariant, but we show that they reduce the RS dependence significantly.

In general the \( \beta \) function includes higher-order perturbative corrections which alter the running of the coupling-constant with respect to the 1-loop evolution. Because of this, PA’s are not exactly invariant under the RS transformation. However, since in QCD with \( N_f = 3, 4 \) or 5, the 1-loop running of the coupling is dominant, PA’s are still almost RS invariant.

The physical significance of the (approximate) RS invariance of PA’s is clear: a part of the contribution of the unknown high orders in a perturbative series is due to diagrams which renormalize the coupling-constant. The numerical importance of these terms is reflected in the RS dependence of the partial-sum. Therefore the fact that PA’s significantly reduce the RS dependence implies that they correctly re-sum these terms. In the large \( \beta_0 \) limit (for example, large \( N_f \) QCD) the arbitrariness in setting the RS can be interpreted as the freedom to replace the gluon propagator by one that is corrected by an arbitrary number of 1-loop insertions. These include both fermion bubbles, and gluon (and ghost) loops. The fact that diagonal PA’s become exactly RS invariant in this limit, suggests that they provide an optimal resummation for this type of higher order corrections (without actually calculating them). Indeed we empirically found \cite{2} that PA’s succeed in predicting higher order coefficients \cite{12,13,14} in the large \( N_f \) limit.

An alternative method to resum higher-order terms that renormalize the coupling constant is the BLM \cite{8} method, where one uses the fact that the leading terms in \( \beta_0 \) can be identified from the leading powers in \( N_f \). One then sets the scale of the leading-order term in the series so that all the known higher-order terms that are leading in \( \beta_0 \) are absorbed. The hope is that also unknown higher-order terms that are leading in \( \beta_0 \) will be accounted for by this choice of scale. Thus we see that at least in the large \( N_f \) limit, PA’s and BLM are very close. Indeed we found that in this limit choosing the BLM scale is mathematically identical to using non-diagonal \( x[0/n] \) PA’s. This equivalence does not hold in the general \( N_f \) case.

A detailed comparison \cite{4} of PA’s with other methods aimed at optimizing perturbative expansions by setting the scale and scheme, such as ECH and PMS has shown that there are no algebraic relations between these two methods and PA’s. On the other hand, good numerical agreement was found in the case of the Bjorken Sum Rule. In this paper we show that this agreement is general, and related to the approximate RS invariance of PA’s.

The paper is organized as follows: In section 2 we introduce the notation and discuss RS dependence in the large-\( \beta_0 \) limit. In section 3 we prove the exact invariance of diagonal PA’s under RS transformations in this limit, and demonstrate it by a simple example. In section 4 we discuss non-diagonal PA’s and show that their RS dependence is reduced as compared to the corresponding partial-sums. Section 5 is devoted to the application of our results to the physical regime of QCD with...
$N_f = 3, 4$ or $5$ flavors. In section 6 we present our physical interpretation of the results and compare the PA method to the ECH, PMS and BLM methods. Section 7 includes our conclusions.

2 RS dependence of observables and the large $\beta_0$ limit

At any order of perturbation theory there remains a residual scale dependence of the order of the next term in the series. Thus, as one goes to higher orders, one expects the scale dependence to decrease. Unfortunately, in practice observables can only be calculated up to some finite (and usually low) order, and thus the theoretical predictions are ambiguous. In QCD observables have so far been calculated only up to next-to-next-to-leading order (at most). Since the coupling-constant in experimentally interesting energies is quite large, this theoretical difficulty becomes a serious problem in comparison of theory with experiment.

The residual RS dependence at a given order is an indication of the importance of higher order corrections, in the sense that they should compensate for this dependence, and therefore their contribution cannot be smaller than the ambiguity introduced by the choice of scale. The actual situation is more complicated, since the ambiguity in the choice of scale is not well-defined: how far a RS can be from the physical scale without introducing new physics? In what renormalization scheme would we define it? and so on. We will not deal here with these well-known open questions any further, but we will make strong use of the RS dependence arguments mentioned above.

Suppose we start with an effective charge\(^{\dagger}\) of an observable $S$ in some renormalizable QFT, calculated up to some order $n + 1$ in perturbation theory in some renormalization scheme and scale,

$$S = x \left(1 + r_1 x + r_2 x^2 + r_3 x^3 + \cdots + r_n x^n\right)$$

In general, both the coefficients $r_i$ and the coupling-constant\(^{\dagger}\) $x = \alpha_s/\pi$ depend on the renormalization scheme and scale. If renormalization is self-consistent then this dependence cancels amongst the different terms in the series, so that the total change in $S$ when changing the scheme or the scale is of order $x \mathcal{O}(x^{n+1})$.

More technically, the coupling-constant $x$ in (2) obeys the Renormalization Group equation.

\(^{\dagger}\)For simplicity we do not deal here with the more general case of $S(x) = x^p(1 + r_1 x + \cdots)$ for $p \neq 1$. The generalization of our results is, however, straightforward.

\(^{\ddagger}\)The notation we use is suitable for QCD, and in some cases we explicitly state QCD results, but the conclusions apply to other QFT’s as well.
Group (RG) equation:

\[ \frac{dx}{dt} = \beta_0 x^2 + \beta_1 x^3 + \beta_2 x^4 + \cdots \equiv \beta(x) \tag{3} \]

where the first two coefficients are the same in any renormalization scheme, while higher coefficients, \( \beta_2, \beta_3, \ldots \) are renormalization scheme dependent. In fact, as was shown in Eq. 4, at any given order in perturbation theory different renormalization schemes can be uniquely defined by these higher coefficients of the \( \beta \) function.

In QCD the first three coefficients of the \( \beta \) function are known [17,18,19]. The first two are:

\[ \beta_0 = -\frac{1}{4} \left( \frac{11}{3} C_a - \frac{2}{3} N_f \right) \tag{4} \]
\[ \beta_1 = \frac{1}{16} \left( -\frac{34}{3} C_a^2 + 2 C_f N_f + \frac{10}{3} C_a N_f \right) \tag{5} \]

where in \( SU(N_c) \) gauge theory \( C_a = N_c \) and \( C_f = (N_c^2 - 1)/(2N_c) \).

We are interested in studying the effect of changing the renormalization scale. Suppose that \( x \) above refers to the coupling-constant being renormalized at the physical scale (for instance, the momentum transfer \( Q^2 \) in deep inelastic scattering), while we denote by \( y \) another legitimate coupling-constant renormalized at some arbitrary scale \( \mu^2 \). We denote by \( t \) the scale shift that corresponds to the transformation from \( x \) to \( y \):

\[ t = \ln \left( \frac{Q^2}{\mu^2} \right) \tag{6} \]

Equation (3) can be integrated order by order to give the required scale-shift transformation:

\[ x = y + \beta_0 t y^2 + \left( \beta_0^2 t^2 + \beta_1 t \right) y^3 + \left( \beta_0^3 t^3 + \frac{5}{2} \beta_1 \beta_0 t^2 + \beta_2 t \right) y^4 + \cdots \tag{7} \]

We turn now to the large \( \beta_0 \) limit, defined by the condition

\[ \beta_0 \gg \beta_i x^i \tag{8} \]

for any \( i \geq 1 \). This is the limit in which our main argument is given. Condition (8) implies that only \( \beta_0^k t^k \) terms in equation (7) are significant. An important example where this condition is realized is QCD with a very large number of flavours (see [14] and the Appendix). Since \( \beta_0 \) is relatively large also in other cases, including in QCD with a few light flavours, this approximation is worth studying. We return to the validity of this approximation in QCD in a later section.

It is important to point out that the question of scheme dependence does not appear in the large \( \beta_0 \) limit, as all the high order coefficients of the \( \beta \) function are not important. Thus the only remaining ambiguity is due the arbitrariness of the
renormalization scale. Therefore, the study of the RS dependence is much simplified in this limit.

When all the higher order terms in the $\beta$ function are neglected, the scale shift transformation (7) simplifies to a geometrical series:

$$ x = y \left( 1 + \beta_0 ty + \beta_0^2 t^2 y^2 + \beta_0^3 t^3 y^3 + \cdots \right) $$

which can be summed to all orders:

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

(9)

In the following we briefly review some properties of this scale shift transformation.

We start by recalling the fact that the transformation (10) admits the following mathematical relation, which we refer to as additivity of scale-shifts:

$$ t_3 = t_1 + t_2 $$

(11)

where

$$ x \xrightarrow{t_1} y \xrightarrow{t_2} z \xrightarrow{t_3} z $$

(12)

This property implies that the set of all transformations (10) with different scale-shifts $t$ forms a group. It is easy to show the existence of a unit operator ($t = 0$), the existence of an inverse transformation ($t \leftrightarrow -t$) and associativity. As for the question of whether the set is a closed one: from the mathematical point of view – it’s clearly not closed, due the the existence of the Landau pole, where the denominator of (10) is zero: $t_{\text{Landau}} = \frac{1}{\beta_0 x}$. From the physical point of view we can assume that the Landau pole is not reached and thus ignore this problem, concluding that RS shifts are indeed a group.

As we will soon be interested in applying transformations like (10) to partial sums and to PA’s, it is important to note here that the transformation (10) is a rational polynomial rather than a polynomial of finite order, and as such, it transforms a polynomial of finite order into a rational polynomial, but transform a rational polynomial into another rational polynomial.

This is a crucial observation which is the basis of the exact RS invariance of diagonal PA’s in the large $\beta_0$ limit, and the reduced RS dependence of non-diagonal PA’s in this limit. It is also the reason why partial sums at a given (finite) order can never be RS invariant.
3 RS invariance of diagonal PA’s in the large $\beta_0$ limit

The statement we prove is that in the large $\beta_0$ limit, starting with a partial sum $S(x)$ of a given order $n + 1$, as in eq. (2), the diagonal $x[N/N + 1]$ PA of $S(x)$, such that $n = 2N + 1$, does not depend on the RS in which the given partial sum was calculated.

The following diagram will be helpful in illustrating our discussion:

```
partial-sum: $S(x) \xrightarrow{t} S_1(y, t) \xrightarrow{t} S_2(x, t)$
\downarrow \quad \downarrow
PA: $P(x) \xrightarrow{t} P_1(y, t) \xrightarrow{t} P_2(x)$
\downarrow \quad \uparrow \quad \uparrow
Taylor of PA: $T(x) \xrightarrow{t} T_1(y, t) \xrightarrow{t} T_2(x)$
```

where $S(x)$ is the $(n+1)$-th order partial sum as in eq. (2), $P(x)$ is the $x[N/N + 1]$ PA constructed from $S(x)$, and $T(x)$ is the infinite-order Taylor series of $P(x)$. The horizontal arrows represent the application of scale-shift transformation according to equation (10), once from $x$ to $y$ (with the scale-shift $t$), and then back, from $y$ to $x$ ($-t$). The first scale-shift in the first line is intentionally represented by a different arrow ($\xrightarrow{\leftarrow}$) than the other scale shifts ($\xrightarrow{}$), meaning that the series in $y$ is truncated at the $(n+1)$-th order after applying the scale-shift transformation. This truncation does not apply to the other scale-shift transformations in the diagram, where an exact transformation according to (10) is meant. In the following we discuss the elements of the above diagram in detail.

The starting point in a resummation process is an $(n+1)$-th order partial-sum which generically can be either $S(x)$ or $S_1(y, t)$. The two partial sums give different numerical results for the observable, but $a\ pri\ or\ one$ is just as good as the other. The numerical difference between $S(x)$ and $S_1(y, t)$ can be calculated by applying the full inverse scale-shift transformation ($-t$) to $S_1(y, t)$ which yields $S_2(x, t)$. The latter is numerically the same as $S_1(y, t)$ but differs from the original $S(x)$ by corrections of order $xO(x^{n+1})$.

---

\(^a\)We take $n$ to be an odd number, in order to construct a diagonal PA.

\(^\dagger\)We remind the reader that in $x[N/N + 1]$ PA we refer to $x$ times a rational polynomial with numerator of order $N$ and a denominator of order $N + 1$, as defined in the Introduction. Therefore we call it a diagonal PA.

\(^*\)In order to calculate $S_1(y)$, one substitutes $x$ as a function of $y$ in $S(x)$ according to (10), and Taylor expands the result to its $(n + 1)$-th order, neglecting all the higher order terms.
Having described the RS dependence of the partial-sums we now consider PA’s. We will now show that diagonal PA’s are RS invariant, i.e. \( P_2(x) \) does not depend on \( t \). We will explicitly show that the two PA’s – \( P(x) \) that is based on \( S(x) \), and \( P_2(x) \) which is calculated by an inverse scale-shift transformation of \( P_1(y, t) \), i.e. based on \( S_1(y, t) \), are exactly equal! This invariance results from the fact that in the large-\( \beta_0 \) limit, RS transformations of the coupling amounts to a homographic transformation of the Padé argument. Diagonal PA’s are known to be invariant under such transformations (see Ref. \[16\] and references therein). The proof is as follows:

a) \( P(x) \) is calculated as the \( x[N/N + 1] \) PA of \( S(x) \):

\[
P(x) = x \frac{1 + a_1 x + ... + a_N x^N}{1 + b_1 x + ... + b_{N+1} x^{N+1}}
\]  

(13)

Similarly, \( P_1(y, t) \) is calculated as the \( y[N/N + 1] \) PA of \( S_1(y, t) \).

b) The scale-shift transformation \([14]\) is applied to \( P(x) \), to give a function which we denote \( P_1^*(y, t) \):

\[
P_1^*(y, t) = \left( \frac{y}{1 - \beta_0 ty} \right) \frac{1 + a_1 \left( \frac{y}{1 - \beta_0 ty} \right) + ... + a_N \left( \frac{y}{1 - \beta_0 ty} \right)^N}{1 + b_1 \left( \frac{y}{1 - \beta_0 ty} \right) + ... + b_{N+1} \left( \frac{y}{1 - \beta_0 ty} \right)^{N+1}}
\]  

(14)

We shall see that \( P_1^*(y, t) \) is equal to \( P_1(y, t) \).

c) By multiplying both the numerator and the denominator by \( (1 - \beta_0 ty)^{N+1} \) we see that \( P_1^*(y, t) \) is actually a a rational polynomial of the type \( y[N/N + 1] \).

d) \( T_1^*(y, t) \) is the Taylor expansion of \( P_1^*(y, t) \). The \( n \) first coefficients of \( T_1^*(y, t) \) are necessarily the same as those in \( S_1(y, t) \). This is because \( T_1^*(y, t) \) can also be viewed as the scale-shifted version of \( T(x) \), which, by the way the \( P(x) \) PA was constructed, has the same \( n \) first coefficients as \( S(x) \). On the other hand, the scale-shift transformation is such that the \( n \) first coefficients of \( T_1^*(y, t) \) (or \( S_1(y, t) \)) depend only on the first \( n \) coefficients in \( T(x) \) (or \( S(x) \)).

e) Since an \( x[N, N + 1] \) PA is uniquely determined by the first \( n \) terms of a power series \( (n = 2N + 1) \), it follows that \( P_1^*(y, t) \) equals to \( P_1(y, t) \).

f) If we now apply an inverse scale-shift \( (-t) \) on \( P_1(y, t) \), we get \( P_2(x) \) which is equal to \( P(x) \) (and therefore does not depend on \( t \)). This is due the existence of an exact inverse scale-shift transformation, or putting it differently, due to additivity of scale-shifts, discussed in the previous section. \[\]

\[\]This additivity of scales breaks down when higher powers of \( t \) are present in the transformation, due to non-negligible higher-order corrections to the \( \beta \) function.
This completes the formal proof of the invariance of PA’s in the large $\beta_0$ limit, as stated at the beginning of the section. We now present a simple example to illustrate how this symmetry works in practice. We start with a fourth order partial-sum ($n = 3$)

$$S(x) = x \left( 1 + r_1 x + r_2 x^2 + r_3 x^3 \right)$$

and calculate $P(x)$ as a $x[1/2]$ PA:

$$P(x) = x \frac{(r_2 - r_1^2) + (2 r_1 r_2 - r_1^3 - r_3) x}{(-r_2^2 + r_1 r_3) x^2 + (-r_3 + r_1 r_2) x + r_2 - r_1^2}$$

Expanding $P(x)$ back in a Taylor series we get $T(x)$:

$$T(x) = x + r_1 x^2 + r_2 x^3 + r_3 x^4 + \frac{r_3^2 - 2 r_2 r_1 r_3 + r_2^2}{r_2 - r_1^2} x^5 + O(x^6)$$

We identify the $r_4$ PAP as the coefficient of $x^5$ in (17).

We calculate the RS dependence of the partial sum $S(x)$ as follows. First, we obtain $S_1(y, t)$ by substituting $x = \frac{y}{1-t\beta_0}$ in $S(x)$, expanding the result into a power series and truncating beyond the $y^4$ term:

$$S_1(y, t) = y + (\beta_0 t + r_1) y^2 + \left( \beta_0^2 t^2 + 2 r_1 \beta_0 t + r_2 \right) y^3 + \left( \beta_0^3 t^3 + r_3 + 3 r_1 \beta_0^2 t^2 + 3 r_2 \beta_0 t \right) y^4$$

We now transform back to $x$ by substituting $y = \frac{x}{1+t\beta_0}$ in $S_1(y, t)$, and expanding to all orders in $x$, to get $S_2(x, t)$. The resulting formula for $S_2(x, t)$ is

$$S_2(x, t) = x + r_1 x^2 + r_2 x^3 + r_3 x^4 + \left( -4 \beta_0^3 t^3 r_1 - \beta_0^4 t^4 - 6 r_2 \beta_0^2 t^2 - 4 r_3 \beta_0 t \right) x^5 + O(x^6)$$

The RS dependence of the partial sum is the difference $\Delta S(x, t)$ between $S_2(x, t)$ and $S(x)$:

$$\Delta S(x, t) \equiv S_2(x, t) - S(x) = \left( -4 \beta_0^3 t^3 r_1 - \beta_0^4 t^4 - 6 r_2 \beta_0^2 t^2 - 4 r_3 \beta_0 t \right) x^5 + O(x^6)$$

We note that the $t$ dependence of $S_2(x, t)$ and thus also $\Delta S(x, t)$ can be quite large for certain values of $t$ (at least for large $t$ it is clear that the contribution due to $\beta_0^4 t^4$ cannot be canceled by other terms). On the other hand, the $x[1/2]$ PA is exactly RS invariant: if we start with the fourth-order partial sum $S_1(y, t)$ of Eq. (18), construct a $y[1/2]$ PA $P_1(y, t)$ and transform back to $x$, we get exactly the $P(x)$ of Eq. (16), as proven.

We stress that also the PAP’s are RS independent. For instance, if we calculate the PA-improved 5-th order partial sum in $y$, and transform it back to the coupling $x$, we will get exactly the same prediction for $r_4$, as in (17), without any $t$-dependence. This is true not only for the PAP of $r_1$ but for any higher-order diagonal PAP.
4 The reduced RS dependence of non-diagonal PA’s in the large $\beta_0$ limit

In the previous section we have proved that diagonal $x[N/N+1]$ PA’s, are exactly RS invariant in the $\beta_0$ limit. In this section we will see that non-diagonal $x[N/M]$ PA’s are not exactly RS invariant even in this limit. However, on the global level (i.e. for large variations of the scale $t$), their RS dependence is much reduced compared to partial sums.

The RS dependence of non-diagonal PA’s is illustrated in the following diagram (cf. analogous diagram in the previous section):

\[
\begin{align*}
\text{partial-sum:} & \quad S(x) \xrightarrow{t} S_1(y, t) \xrightarrow{-t} S_2(x, t) \\
\downarrow & \quad \downarrow \\
\text{PA:} & \quad P(x) \xrightarrow{t} P_1^*(y, t) \neq P_1(y, t) \\
\downarrow & \quad \uparrow \\
\text{Taylor of PA:} & \quad T(x) \xrightarrow{t} T_1(y, t) \xrightarrow{-t} T_2(x, t)
\end{align*}
\]

To illustrate this, we turn now to the simplest example, where we start with a third order series ($n = 2$):

\[S(x) = x \left(1 + r_1 x + r_2 x^2\right)\tag{21}\]

Calculating its $x[1/1]$ PA, we get

\[P(x) = x \frac{r_1 + (r_1^2 - r_2) x}{r_1 - r_2 x}\tag{22}\]

Expanding back in a Taylor series we obtain:

\[T(x) = x + r_1 x^2 + r_2 x^3 + \frac{r_2^2}{r_1} x^4 + O(x^5).\tag{23}\]

Applying the scale shift transformation to $S(x)$ yields:

\[S\left(y \frac{1}{1 - t \beta_0 y}\right) = y \left(1 + \frac{r_1 y}{1 - \beta_0 t y} + \frac{r_2 y^2}{(1 - \beta_0 t y)^2}\right)\frac{1}{1 - \beta_0 t y}\tag{24}\]

which can be Taylor expanded in $y$, and truncated at fourth order, to give:

\[S_1(y, t) = y + (r_1 + \beta_0 t) y^2 + \left(2 r_1 \beta_0 t + r_2 + \beta_0^2 t^2\right) y^3\tag{25}\]
Constructing a $y[1/1]$ PA, we get:

$$ P_1(y, t) = y \frac{(r_1 + \beta_0 t) + (r_1^2 - r_2) y}{(-2 r_1 \beta_0 t - r_2 - \beta_0 t^2)} y + r_1 + \beta_0 t $$

(26)

On the other hand, if we transform $P(x)$ to $y$, using the exact scale-shift transformation (24), we get:

$$ P^*_1(y, t) = y \frac{r_1 + (r_1^2 - r_1 \beta_0 t - r_2) y}{r_1 - (r_2 + 2 r_1 \beta_0 t) y + (r_2 + r_1 \beta_0 t) \beta_0 t y^2} $$

(27)

We see that $P^*_1(y, t)$ is a diagonal rational polynomial, of type $y[1/2]$, rather than an off-diagonal rational polynomial of the type $y[1/1]$, like $P_1(y, t)$ of Eq. (24). Therefore $P^*_1(y, t) \neq P_1(y, t)$, and the scale invariance property does not hold here.

In order to measure the RS dependence of the non-diagonal PA, we define $\Delta T(x, t)$, in analogy with $\Delta S(x, t)$ which was introduced in Eq. (24) to measure the RS dependence of partial-sums.

$$ \Delta T(x, t) \equiv T_2(x, t) - T(x), $$

(28)

where as $T(x)$ is the Taylor expansion of $P(x)$ and $T_2(x, t)$ is obtained by applying an inverse transformation ($-t$) to the PA-improved partial sum $T_1(y, t)$, the Taylor expansion of $P_1(y, t)$ (see diagram).

Going back to our example, we calculate $T_2(x, t)$,

$$ T_2(x, t) = x \left[ 1 + r_1 x + r_2 x^2 + \frac{-\beta_0 t^2 r_2 + r_2 \beta_0 t r_2 + r_1 r_2 \beta_0 t^2}{\beta_0 t + r_1} x^3 + \mathcal{O}(x^4) \right] $$

(29)

As expected, up to $r_2$ we obtain the same coefficients we started with. The predicted $r_3$ turns out to be scale dependent (and therefore different from the one obtained from $P(x)$). Thus for the RS dependence of the PA function $\Delta T(x, t)$ we obtain:

$$ \Delta T(x, t) = \left( \frac{-\beta_0 t^2 r_2 + r_2 \beta_0 t r_2 + r_1 r_2 \beta_0 t^2}{\beta_0 t + r_1} - \frac{r_2^2}{r_1} \right) x^4 + \mathcal{O}(x^5) $$

(30)

This has to be compared with the RS dependence of the partial sum. Taking the inverse ($-t$) transformation of $S_1(y, t)$ we get $S_2(x, t)$:

$$ S_2(x, t) = x + r_1 x^2 + r_2 x^3 + \left( -\beta_0 t^3 - 3 r_1 \beta_0^2 t^2 - 3 r_2 \beta_0 t \right) x^4 + \mathcal{O}(x^5) $$

(31)

and therefore:

$$ \Delta S(x, t) = \left( -\beta_0 t^3 - 3 r_1 \beta_0^2 t^2 - 3 r_2 \beta_0 t \right) x^4 + \mathcal{O}(x^5) $$

(32)

Comparing $\Delta T(x, t)$ with $\Delta S(x, t)$ we make the following observations:
a) The asymptotic behavior of $\Delta T(x, t)$ at large scale variations (large $t$), is much milder than that of $\Delta S(x, t)$

$$
\Delta T(x, t) \sim (r_1^2 - r_2)\beta_0 t x^4 + O(x^5)
$$

vs.

$$
\Delta S(x, t) \sim -\beta_0^3 t^3 x^4 + O(x^5)
$$

b) On the other hand, there is a pole in $\Delta T(x, t)$. At certain scales it results in very large deviations of the PA from the value typical at most other scales. We thus have to be careful not to use the $x[1/1]$ PA at these scales (for any specific case one can plot the $x[1/1]$ PA as a function of the RS, and identify the scales that are badly influenced by the pole).

We now turn to a second example, where we construct a $x[0/2]$ PA from the same partial sum (21). In this case we do not give all the details, but only state the final result for $\Delta T(x, t)$:

$$
\Delta T(x, t) = 
\left[ -\beta_0 t(r_1^2 - r_2) + 2r_2 r_1 - r_3 \right] x^4 + O(x^5)
$$

We notice that for the $x[0/2]$ PA (as for the $x[1/1]$ PA) the asymptotic behavior is mild, but (in contrast to the $x[1/1]$ PA) no poles appear in $\Delta T(x, t)$. Thus we conclude that the $x[0/2]$ PA is much less scale dependent than either the partial sum or the $x[1/1]$ PA.

An interesting result is that the asymptotic behavior of $\Delta T(x, t)$ for large enough $t$ in the case of the $x[0/2]$ PA is the same as that of the $x[1/1]$ PA. This can be confirmed by comparing the large $t$ behavior of Eq. (30) and Eq. (35). The mathematical reason for this similarity is that in both cases, the non-diagonal PA’s transform under the scale-shift transformation into diagonal rational polynomials of order 2 ($x[1/2]$ PA). Since we lack one parameter ($r_3$) in order to write a “correct” $x[1/2]$ PA to describe the observable, we are left with some ambiguity, having a full set of functions of the type $x[1/2]$ with coefficients that depend on one free parameter ($r_3$) rather than one specific $x[1/2]$ PA. The remaining ambiguity is reflected both in the freedom to choose among the $x[1/1]$ and $x[0/2]$ PA’s, and in the freedom to set the RS. The interpretation of this result is that the choice between $x[1/1]$ and $x[0/2]$ PA is equivalent to the choice between different RS’s. We will later see how this generalizes to higher-orders.

Note that throughout the analysis we did not make any specific assumptions about the perturbative coefficients $r_i$ of the observable under consideration. In [4] we examined the $[1/1]$ and $[0/2]$ PA’s considered here, as well as the partial sum, for the physical example of the Bjorken Sum Rule with $N_f = 3$. We found that indeed the RS dependence of the $x[0/2]$ PA is much reduced as compared to the partial sum. We also found that the $x[1/1]$ PA has a large RS dependence in specific RS’s. We now see, in retrospective from the large $\beta_0$ limit, that these features are
general. In the next section we will show why the large $\beta_0$ assumption is a good approximation for QCD with 3 flavours. But before doing so, we want to see how the present conclusions for the $n = 2$ case can be generalized to higher $n$.

For $n = 3$, we start with a partial sum as in Eq. (15). We can construct two non-diagonal PA's: $x[2/1]$ and $x[0/3]$, in addition to the diagonal $x[1/2]$ PA studied in detail in the previous section. We found that the partial sum has a considerable RS dependence, as described by (20), while the $x[1/2]$ PA is exactly RS invariant. Here we look on $\Delta T(x,t)$ for the $x[2/1]$ and $x[0/3]$ PA’s.

The asymptotic behavior of $\Delta T(x,t)$ at large scale shifts is the same for $x[2/1]$ and $x[0/3]$ PA’s:

$$\Delta T(x,t) \sim (r_1^2 - r_2)\beta_0^2 t^2 x^5 + O(x^6)$$  \hspace{1cm} (36)

to be compared with the asymptotic behavior of $\Delta S(x,t)$ from equation (20):

$$\Delta S(x,t) \sim -\beta_0^4 t^4 x^5 + O(x^6)$$  \hspace{1cm} (37)

$\Delta T(x,t)$ for the $x[2/1]$ PA has poles (the coefficient of $x^5$ has two poles in $t$), whereas $\Delta T(x,t)$ for the $x[0/3]$ PA does not. This makes the use of the $x[0/3]$ PA much safer than the use of the $x[2/1]$ PA. However, here it is preferable to use the diagonal $x[1/2]$ PA which is exactly invariant and therefore the other two will not be relevant.

For $n = 4$ we have four non-diagonal PA’s: $x[3/1]$, $x[2/2]$, $x[1/3]$ and $x[0/4]$. The asymptotic behavior of $\Delta T(x,t)$ for $x[3/1]$ and $x[0/4]$ PA’s is the same, and the leading term is proportional to $\beta_0^3 t^3 x^6$; the asymptotic behavior of $\Delta T(x,t)$ for $x[2/2]$ and $x[1/3]$ PA’s is again the same, and the leading term is proportional to $\beta_0 t x^6$. These are to be compared to the asymptotic behavior of the RS dependence of the partial sum ($\Delta S(x,t)$) in which the leading term is $\beta_0^5 t^5 x^6$. Out of the four PA’s, only $x[0/4]$ does not have poles in $\Delta T(x,t)$.

Generally, starting with a partial sum of order $n+1$ and constructing an $x[N/M]$ PA ($N + M = n$), we find the asymptotic behavior of

$$\Delta T(x,t) \sim \beta_0^d t^d x^{n+2}$$  \hspace{1cm} (38)

where $d$ is given by:

$$d = |N + 1 - M| = |2N + 1 - n|$$  \hspace{1cm} (39)

while the asymptotic behavior of $\Delta S(x,t)$ is

$$\Delta S(x,t) \sim \beta_0^{n+1} t^{n+1} x^{n+2}$$  \hspace{1cm} (40)

d actually measures the dimensionality of the ambiguity space (= number of unknown parameters) that exists in writing a diagonal $x[N/N+1]$ PA (for $N \geq M$) or $x[M - 1/M]$ PA (for $N < M - 1$) describing the series. It’s clear that $d < n + 1$
and therefore the global RS dependence of the $x[N/M]$ PA is milder than that of the partial sum. On the other hand, already at the leading term in $\Delta T(x,t)$ there will be $N$ poles which will cause specific RS’s to exhibit sharp scale dependence, something that we want to avoid. Only the $x[0/n]$ PA will not have any poles in $\Delta T(x,t)$.

We conclude that in general non-diagonal PA’s also have a reduced RS dependence as compared to the partial-sum. In [4] we recommended considering the RS dependence in choosing the appropriate PA. The above discussion shows that in cases where the large $\beta_0$ approximation is valid, for series of even orders in the coupling-constant (odd $n = 2N + 1$), the diagonal $x[N/N + 1]$ PA’s should be preferred, while for odd orders in the coupling (even $n = 2N$), the next to diagonal PA’s ($x[N/N]$ and $x[N - 1/N + 1]$) are best from the point of view of the global RS dependence, while the $x[0/n]$ PA is the only one in which poles in $\Delta T(x,t)$ are guaranteed not to appear, and thus likely to exhibit the least RS dependence for small scale variations.

5 Applicability of the results for QCD with $N_f = 3, 4$ or $5$

In this section we leave the large $\beta_0$ limit and consider the physical example of QCD with 3, 4 or 5 quark flavors.

As mentioned in the Introduction, we already have strong evidence [2,3,4] that PA’s are useful in this case. Moreover we showed in [4] that $x[0/2]$ PA significantly reduces the RS dependence of the Bjorken Sum Rule in any renormalization scheme. Therefore we already know that the results we presented here for the large $\beta_0$ limit are approximately true also in real-world QCD, at least for the example of the Bjorken sum rule. In this section we will show that the approximate invariance of PA’s under RS transformations holds for a generic QCD observable in a wide range of renormalization schemes. Actually, we believe that this approximate invariance holds in many QFT examples, since the only requirement is that the running of the relevant coupling will be dominated by the 1-loop contribution.

In general, the scale-shift transformation (7) cannot be written in the form (10), since higher order terms in the $\beta$ function do not vanish. In fact, the problem becomes even more complicated because the generic scale-shift transformation is not well defined, since it can only be written as a divergent asymptotic series, and might not even be Borel-sumable, due to IR renormalons. In addition to the RS dependence, there is also renormalization scheme dependence, which can be viewed as arbitrariness in setting the higher order coefficients of the $\beta$ function. This makes it clear that the results of RS invariance in the large $\beta_0$ limit cannot be formally extended to the general case.
On the other hand, we can check to what extent the scale-shift transformation which is exact in the large $\beta_0$ limit can serve as an approximation to the actual scale-shift in the general case (4). Let’s consider the first two terms in (7) which deviate from (10) – these are the third and the fourth orders in $y$:

$$\beta_0^2 t^2 \rightarrow \beta_0^2 t^2 + \beta_1 t$$

$$\beta_0^3 t^3 \rightarrow \beta_0^3 t^3 + \frac{5}{2} \beta_1 \beta_0 t^2 + \beta_2 t$$ (41)

In order to measure the effect of these higher-order terms we define:

$$C_1(t) = \frac{\beta_0^2 t^2 + \beta_1 t}{\beta_0^2 t^2}$$ (42)

and

$$C_2(t) = \frac{\beta_0^3 t^3 + \frac{5}{2} \beta_1 \beta_0 t^2 + \beta_2 t}{\beta_0^3 t^3}$$ (43)

We see that for any (non-zero) $\beta_0$ and large enough scale shift $t$, the dominance of the leading $\beta_0^k t^k$ terms is recovered.

Since we are interested specifically in QCD with $N_f = 3$, 4 and 5, we can numerically estimate the dominance of the leading $\beta_0^k t^k$ terms. For instance, for $N_f = 3$ we have in the $\overline{\text{MS}}$ renormalization scheme [17,18,19]: $\beta_0 = -2.25$, $\beta_1 = -4$ and $\beta_2 = -10.06$. Using these values we calculate $C_1(t)$ and $C_2(t)$ and look at the actual transformation of the coupling as a function of $t$.

In Figure 1 we plot $y(t)$ for $x \equiv \alpha_s/\pi = 0.07$, corresponding to $Q^2 = 20 \text{ GeV}^2$ in $\overline{\text{MS}}$ with $\mu^2 = Q^2$. We calculate $y(t)$ in three different ways:

a) The exact transformation in the large $\beta_0$ limit:

$$y(t) = \frac{x}{1 + \beta_0 t x}$$ (44)

b) The first four terms in the leading $\beta_0$ transformation.

$$y(t) = x - \beta_0 t x^2 + \beta_0^2 t^2 x^3 - \beta_0^3 t^3 x^4$$ (45)

(the difference between (45) and (44) at large $t$ is due to higher orders).

c) The first four terms in the QCD RS transformation, with $N_f = 3$ ($\beta_2$ taken in $\overline{\text{MS}}$).

$$y(t) = x - \beta_0 t x^2 + C_1(-t) \beta_0^2 t^2 x^3 - C_2(-t) \beta_0^3 t^3 x^4$$ (46)

Figure 2 presents the corresponding relative deviations of the the leading $\beta_0$ transformations (44) and (45) from the QCD transformation (46).

From figures 1 and 2 we see that the leading $\beta_0$ approximation is quite accurate for QCD with 3 flavours in a very large range of scales. We also find that already
at $|t| \gtrsim 4$ the error due to the neglected higher order terms becomes larger than the one due to neglecting of $\beta_1$ and $\beta_2$.

The numerical results for $N_f = 4, 5$, as well as for other renormalization schemes (i.e. other values of $\beta_2$) are almost identical to those presented in figures [1] and [2].

The conclusion from this analysis is that the scale-shift transformation in QCD with $N_f = 3, 4$ or 5 can be well approximated by the large $\beta_0$ scale-shift transformation of (44). Therefore, to a good approximation, the conclusions we drew concerning the invariance of PA’s in the large $\beta_0$ limit apply in the realistic case as well. As mentioned, we already found through an explicit calculation [1], that $x[0/2]$ PA reduces the RS dependence of the Bjorken Sum Rule in wide range of renormalization schemes.

6 The physical interpretation and comparison with ECH, PMS and BLM

In the previous sections we showed that diagonal PA’s become RS invariant in the limit of large $\beta_0$, while non-diagonal PA’s generally reduce the RS dependence of the observable. Since the leading $\beta_0$ approximation is good in many physical cases, including QCD, PA’s have a much reduced RS dependence there as well. In this section we discuss the physical interpretation of this result and compare the PA method to the ECH, PMS and BLM methods.

6.1 Physical interpretation

In general, a significant part of the contribution of unknown higher orders in a perturbative series is due to diagrams that renormalize the coupling-constant. The numerical importance of these terms is reflected in the RS dependence of the partial-sum since it is the higher order terms that compensate for this unphysical dependence.

In order to understand the meaning of the (approximate) RS independence of PA’s, we first analyze it in the large $\beta_0$ limit, where the running of the coupling-constant is completely determined by a 1-loop renormalization.

We found that in this limit diagonal PA’s become exactly RS invariant. This strongly implies that the diagonal PA sums-up the higher order contributions that compensate for the RS dependence of the corresponding partial-sum.

On the other hand, even in the large $\beta_0$ limit, we do not expect the diagonal PA to sum the higher order terms exactly. This is because rational functions cannot represent factorial behavior of the coefficients as expected at large orders due to
renormalons.

All order perturbative calculations for some observables in QED and QCD in the large $N_f$ limit have been performed (see for instance [12] and [13]). The conditions for the dominance of the 1-loop running of the coupling-constant (8) hold in this limit (see the Appendix), and therefore our conclusions concerning the RS independence of diagonal PA’s hold as well. Thus this limit provides a good testing ground for our method. In the large $N_f$ limit only fermion-bubble renormalon chains contribute at high orders, and therefore the results are extremely simple in the Borel plane. The only remaining ambiguity is related to the integration through poles located on the positive real axis in the Borel plane, i.e. the IR renormalons in QCD (and UV renormalons in QED). After performing the integration and going back to the $\alpha_s$ plane, we do not get a rational polynomial in $\alpha_s$. Therefore PA’s in the $\alpha_s$ plane cannot be expected to give the “exact” result, but only to provide good approximations, and “converge” with increasing order‡.

Since the RS independence of PA’s in the large $\beta_0$ limit is exact, we suspect that diagonal PA’s, although do not sum the full series, do provide some kind of optimal resummation of higher order corrections. We expect, for instance, that in the large $\beta_0$ limit diagonal PA’s are more accurate than any other non-diagonal PA and at least as accurate as any scale-setting method. We show later that in the large $N_f$ limit, choosing the BLM scale is equivalent to using the $x[0/n]$ non-diagonal PA.

Given the RS independence of PA’s, it is interesting to examine numerically the convergence of increasing order PA’s and the precision of the Padé Approximant predictions (PAP’s) as compared to exact calculations in the large-$N_f$ limit. An empirical study of this kind has been done in [2] and [3]. It was found that increasing order PA’s do not converge but oscillate around the Cauchy Principal-Value of the inverse Borel integral. These oscillations are due to IR renormalons and in the absence of such, increasing order PA’s converge to the Borel sum of the asymptotic series. It was also found that increasing order PAP’s become very close to the exact perturbative coefficients, and that the errors decrease exponentially with order. The errors can be approximated by a simple function, and thus a further increase in the PAP precision is possible (this issue has been discussed in [3] and in [15]).

We stress that the exact RS independence of diagonal PA’s (and the reduced dependence of non-diagonal PA’s) holds whenever the 1-loop running of the coupling is dominant (cf. Eq. (8)). Large $\beta_0$ does not necessarily imply large $N_f$, as there may be many other cases in QFT where the condition (8) holds. As we saw in the previous section, the large $\beta_0$ approximation is quite good in QCD with only 3 to 5 flavours. However, in contrast with QED, the 1-loop running of the coupling in QCD is dominated by gluon (and ghost) loops and not by fermion loops. The BLM method resums 1-loop insertions that renormalize the coupling-constant. Therefore

‡We use quotation marks to indicate that the terms are not well defined mathematically (due to the existence of singularities on the integration path).
it is natural to compare the PA and BLM methods, as we do in Sec. [6.3].

We see that the basic physical idea behind PA’s, and the scale and scheme setting methods is the same: part of the contribution of unknown higher order corrections is related to the running of the coupling constant. Thus it may be possible improve the perturbative result through resumming part of these unknown terms by relying on the characteristics of the renormalization group. In the following subsections we compare the PA method to ECH, PMS and BLM.

6.2 Comparison of PA’s with ECH and PMS

The method of Effective Charges (ECH) [3] is based on choosing the renormalization scale and scheme, such that the series reduces to a leading order term (all the other known coefficients in this scheme are exactly zero). There is a unique scheme that fulfills this criterion.

In [4] we found good numerical agreement between $x[0/2]$ PA of the Bjorken sum-rule (which turned out to be almost RS invariant), and the ECH (and PMS) scheme-setting methods. As shown in [4], there seems to be no algebraic relation between these two methods and the PA. Still, our results in this paper imply that the numerical agreement is general. The reason is quite simple, and it is directly related to the approximate RS independence of the PA’s. Suppose a PA was exactly scale and scheme invariant. Then we would get exactly the same numerical result in any scheme and scale, and in the ECH in particular. However, in the ECH scheme, the series reduces to a leading order term (all the higher order coefficients are exactly zero) and therefore the PA is identical to the “partial sum”. Therefore the ECH result is exactly equal to PA in any scale and scheme. Of course, this exact agreement breaks down as effects of RS dependence are turned on; these include the possible choice of a non-diagonal PA, higher order corrections to the $\beta$ function, and scheme dependence. Still, we expect that at scales and schemes not too far from ECH, the PA result will be much closer to the ECH result than to the corresponding partial-sums.$^\S$

Another approach to set the scale and scheme is the Principle of Minimal Sensitivity [5]. In this method, one chooses the scheme in which the renormalization scheme and scale dependence vanishes exactly. PMS is close to ECH both in its nature, and in it’s numerical predictions (see [4] and [1]). Knowing now that ECH and PA’s methods generally agree, we also expect PMS to be close to PA’s. We note that reducing the RS dependence is the common basis for both PA’s and PMS. The difference is that PA’s can be applied at any scale and scheme and they reduce the RS dependence globally (even for large scale variations), while PMS chooses a scale and scheme such that the local scale dependence vanishes.

$^\S$This is true as long as pole effects of non-diagonal PA’s are avoided.
6.3 Comparison between PA’s and BLM

The BLM method is based on the observation that in the large-$N_f$ limit of QCD all the higher-order corrections are due to fermion loops, which are also responsible for the running of the coupling. Therefore they can be absorbed by changing the RS at which the coupling is defined. It is reasonable to expect that absorbing these corrections in the scale will improve the perturbative result.

In QCD with only a few flavours, one can use the fact that $\beta_0$ is linear in $N_f$ to single out the 1-loop corrections to the coupling by identifying the terms that are leading in $N_f$. Thus also in QCD 1-loop corrections to the coupling can be absorbed by setting the scale of the leading term. Technically this is done by setting the scale so that at higher orders all the leading terms in $N_f$ will cancel exactly.

BLM was generalized to account for non-leading corrections to the renormalization of the coupling in several ways (see, for instance, [10], [9] and [11]). Since the basic intuition of BLM and its generalizations relies on the large $N_f$ limit, we present a detailed comparison with PA’s for this case only.

We start with an effective charge of a generic observable in the large $N_f$ limit (see the Appendix). The BLM scale-setting procedure is based on eliminating the $N_f$ dependence of the coefficients $r_i$. In the large $N_f$ limit this results in complete elimination of the $r_i$’s, since in this limit $r_i \propto N_f^i$ (there are no sub-leading terms), leading to the result:

$$S_{BLM} = x(t_{BLM})$$

or, equivalently, using the large $N_f$ limit notation in the Appendix:

$$S_{BLM}^{N_f \to \infty} = z(t_{BLM})$$

where $z \equiv xN_f$ and

$$t_{BLM} = t_1 + t_2 z + t_3 z^2 + \cdots + t_n z^{n-1}$$

where $t_1$ is proportional to $r_1$, $t_2 = t_2(r_1, r_2)$, $t_3 = t_3(r_1, r_2, r_3)$, etc.

The leading-order BLM scale $t_1$ is chosen such that $c_1$ (or $r_1 \equiv c_1 N_f$) is eliminated. Using this scale results in a summation of the leading diagrams which correct the gluon propagator at higher orders. For instance, a contribution like $c_1^2 z^3$ (or $r_1^2 x^3$) is accounted for (cf. (A.3)), although terms of order $z^3$ were not initially included.

In order to eliminate also the next coefficient $c_2$, one has to alter the scale-shift by adding a term $t_2 z$ that is proportional to the coupling. Similarly, one adds $t_3 z^2$ to eliminate $c_3$, and so on. In such a way all the known terms can be absorbed.

\footnote{We will later discuss the effects of the non-leading corrections to $t_{BLM}$.}
into the definition of the coupling-constant, hopefully summing correctly the bulk of higher-order unknown contributions.

Several different proposals were made for generalizing BLM beyond the leading scale $t_{BLM} = t_1$, but in the large $N_f$ limit they all agree: both the single-scale BLM method of Ref. [9] and the multi-scale method of Ref. [10] reduce then to (18) and (19).

Suppose we want to calculate the effective charge in the large $\beta_0$ limit by the BLM prescription, according to (48) and (49), assuming the coupling-constant at the physical scale (i.e. $z$) is known. The effective charge we are calculating is just the coupling-constant at the scale $t_{BLM}$, given by the inverse of relation (A.6):

$$S_{BLM}^{N_f \to \infty}(z) = \frac{z}{1 + \beta_0 t_{BLM} z}$$

where from now on $\beta_0$ stands for to $\beta_0^{N_f \to \infty} = \frac{1}{6}$. We substitute (19) into (50) to get:

$$S_{BLM}^{N_f \to \infty}(z) = \frac{z}{1 + \beta_0 t_1 z + \beta_0 t_2 z^2 + \cdots + \beta_0 t_n z^n}$$

By construction, if $S_{BLM}^{N_f \to \infty}(z)$ is expanded in powers of $z$ up to order $n + 1$, one would get the original series $S(z)$. We note that the r.h.s. of (51) is a $z[0/n]$ rational polynomial. Now, since there is a unique $z[0/n]$ PA which has an $(n+1)$-th order Taylor expansion equal to $S(z)$, we conclude that in the large $N_f$ limit BLM is exactly equivalent to $z[0/n]$ PA’s.

In view of this result it is worthwhile to repeat the characteristics of the $z[0/n]$ functions, found in Section 4:

a) As other non-diagonal PA’s, a $z[0/n]$ PA does depend on the RS. The leading term in this RS dependence is proportional to $\beta_0^{n-1} t^{n-1}$, significantly less than $\beta_0 t^{n+1}$ in the partial-sum.

b) As opposed to other non-diagonal PA’s, the $z[0/n]$ PA is strictly free from any poles in its RS dependence.

We wish to emphasize that the BLM prescription beyond the leading order (i.e. beyond $t_{BLM} = t_1$) cannot be regarded as a choice of RS in the strict sense, since terms that depend on $z$ in (19) break the additivity of scale-shifts in the transformation (A.6). Putting it differently: after substituting $t_{BLM}$ in (A.6), $w$ depends on $\parallel$This consensus does not include the method described in [1] where $t_{BLM} = t_1$ at any order. In this method the higher order terms in $(\beta_0 x)$ as well as effects due to sub-leading running of the coupling are resummed by setting the higher orders of the $\beta$ function, i.e. choosing the renormalization scheme such that the remaining coefficients reach their conformal-limit value. This idea cannot be applied in the large $N_f$ limit, where one neglects the higher order corrections to the $\beta$ function altogether.\end{footnote}
z in a more complex way than implied by the RS transformation. This is why the BLM result is not free of RS dependence and is not equivalent to a diagonal PA \(^{*}\). This does not apply to the simplest case of a next-to-leading order series, where \(t_{BLM} = t_1\). Here, BLM in the large \(N_f\) limit becomes simply a \(x[0/1]\) PA, which is RS invariant.

We wish to stress that the equivalence of \(x[0/n]\) PA’s and BLM is of course true only in the large \(N_f\) limit. Moreover, \(x[0/n]\) PA’s are different from all the various generalization of BLM that attempt to take into account effects due to non-leading running of the coupling-constant. If one wishes, one can regard \(x[0/n]\) PA’s as another generalization of this kind.

7 Conclusions

We showed that in the \(\beta_0\) limit diagonal PA’s of perturbative series become exactly renormalization scale independent.

This implies that diagonal PA’s are correctly resumming contributions from higher order diagrams which are responsible for the renormalization of the coupling-constant.

Non-diagonal PA’s are not exactly invariant even in the large \(\beta_0\) limit, but still reduce the global RS dependence as compared to partial-sums. Among the different non-diagonal PA’s, the only one that has a completely regular behavior with respect to scale variations is the \(x[0/n]\) PA. We have shown that in the large \(N_f\) limit of QCD, the latter is identical to the BLM scale-setting procedure.

In physical cases, higher order corrections in the \(\beta\) function break the RS independence of PA’s, introducing a small scale and scheme dependence, even for diagonal PA’s.

We also showed that PA’s, when they are indeed RS invariant to a good approximation, lead to the same numerical result as the ECH method.

An important feature of PA’s (one that in our view makes them more useful than scale and scheme setting methods) is simply that they can be used in any scale and scheme. The comparison of results in different scales and schemes can then serve two goals:

a) Estimate the reliability of the PA method is in each particular case, by considering the scale and scheme dependence of the partial sum as a reference, as was done for the Bjorken sum rule in Ref. [4].

\(^{*}\)The argument we used in subsection 6.2 to show the agreement between ECH and PA’s does not apply in the case of BLM in the large \(N_f\) limit, even though the series reduces to a single term. The reason is precisely the fact that BLM is not strictly a choice of RS.
b) Use the residual scale and scheme dependence as a lower bound for the theoretical error.

Finally, we feel that the “surprising success” of PA’s in QCD, and generally in QFT, is now based on a much more firm basis.

Acknowledgements

I thank Marek Karliner and John Ellis for very useful discussions. The research was supported in part by the Israel Science Foundation administered by the Israel Academy of Sciences and Humanities, and by a Grant from the G.I.F., the German-Israeli Foundation for Scientific Research and Development.
Appendix - The large $N_f$ limit

In this Appendix we briefly present some of the basic formulae that are used in the large $N_f$ limit calculations. This concerns the discussion in section 6 and especially subsection 6.3 where we compare PA’s and BLM in this limit.

Starting with (2) and using the fact that the leading term in $r_i$ is proportional to $N_f^i$, we obtain:

$$S(x) = x \left(1 + r_1 x + r_2 x^2 + r_3 x^3 + \cdots + r_n x^n \right)$$

(A.1)

We define $z \equiv x N_f$ and $S^{N_f \to \infty}(z) = S(x) N_f$ and thus:

$$S^{N_f \to \infty}(z) = z \left(1 + c_1 z + c_2 z^2 + c_3 z^3 + \cdots + c_n z^n \right)$$

(A.2)

In the same manner we change the notations for the $\beta$ function (3):

$$\frac{dz}{dt} = \beta_0 N_f z^2 + \beta_1 N_f^2 z^3 + \beta_2 N_f^3 z^4 + \cdots$$

(A.3)

Remembering that $\beta_0 \sim N_f$ while at higher orders $\beta_i \sim N_f^i$ (cf. (4) and (5)), we conclude that higher order corrections to the $\beta$ function are negligible, being sub-leading in $N_f$, and (A.3) can be written as:

$$\frac{dz}{dt} = \beta_0^{N_f \to \infty} z^2$$

(A.4)

where $\beta_0^{N_f \to \infty} = \frac{1}{6}$. Therefore Eq. (4) translates into:

$$z = w + \beta_0^{N_f \to \infty} t w^2 + \left(\beta_0^{N_f \to \infty}\right)^2 t^2 w^3 + \left(\beta_0^{N_f \to \infty}\right)^3 t^3 w^4 + \cdots$$

(A.5)

where $w$ is the coupling-constant that is defined at the new renormalization point $\mu$ (see Section 2). Finally, Eq. (10) translates into:

$$z = \frac{w}{1 - \beta_0^{N_f \to \infty} t w}$$

(A.6)


References

[1] M.A. Samuel, G. Li and E. Steinfelds, Phys. Rev. D48 (1993) 869 and Phys. Lett. B323 (1994) 188; M.A. Samuel and G. Li, Int. J. Th. Phys. 33 (1994) 1461 and Phys. Lett. B331 (1994) 114.

[2] M.A. Samuel, J. Ellis and M. Karliner, Phys. Rev. Lett. 74 (1995) 4380.

[3] J. Ellis, E. Gardi M. Karliner and M.A. Samuel, Phys. Lett. B366 (1996) 268.

[4] J. Ellis, E. Gardi M. Karliner and M.A. Samuel, Phys. Rev. D54 (1996) 6986.

[5] P.M. Stevenson, Phys. Rev. D23 (1981) 2916.

[6] G. Grunberg Phys. Rev. D29 (1984) 2315.

[7] A.L. Kataev and V.V. Strashenko Mod. Phys. Lett. A10 (1995) 235.

[8] S.J. Brodsky, G.P. Lepage and P.M. Mackenzie, Phys. Rev. D28 (1983) 228;

[9] G. Grunberg and A.L. Kataev Phys. Lett. B279 (1992) 352-358

[10] S.J. Brodsky and H.J. Lu, Phys. Rev. D51 (1995) 3652.

[11] J. Rathsman, Phys. Rev. D54 (1996) 3420.

[12] D.J. Broadhurst, Z. Phys C58 (1993) 339

[13] M. Beneke and V.M. Braun, hep-ph/9411229

[14] C.N. Lovett-Turner and C.J. Maxwell, Nucl. Phys. B432 (1994) 147.

[15] J. Ellis, M. Karliner, M.A. Samuel, in preparation.

[16] George A. Baker, Jr. and Peter Graves-Morris, Padé Approximants, Volume 13 of the Gian-Carlo Rota Encyclopedia of Mathematics and it’s Applications. Eddison-Wesley Publishing Company, 1981.

[17] C.J. Gross, F. Wilczek, Phys. Rev. Lett. 30 (1973) 1343; H.D. Politzer, Phys. Rev. Lett. 30 (1973) 1346.

[18] W.E. Caswell, Phys. Rev. Lett 33 (1974) 244; D.R.T Jones, Nucl. Phys. B75 (1974) 531.

[19] S. A. Larin and J. A. Vermaseren Phys. Lett. B303 (1993) 334-336.
Figure 1: $y(t)$ as a function of the scale-shift for QCD with 3 flavours, as calculated in three different ways: (a) all-order resummation of the leading $\beta_0$ terms (continuous line), (b) first four terms in the leading $\beta_0$ approximation (dashed line), and (c) the first four terms in the actual QCD scale-shift transformation (dotted line).
Figure 2: The relative deviation of the leading $\beta_0$ approximations for $y(t)$ from the QCD transformation, given by (46). The continuous line represents the relative deviation of the all-order resummation of the leading $\beta_0$ terms (44), while the dashed line stands for the relative deviation of the first four terms in the leading $\beta_0$ transformation (43).