Light-quark masses and renormalons

A.L. Kataev

Theoretical Physics Division, CERN CH-1211, Geneva 23, Switzerland
and Institute for Nuclear Research of the Academy of Sciences of Russia,
117312 Moscow, Russia

ABSTRACT

A brief review of the problem of the determination of light-quark masses from QCD sum rules for the correlators of scalar and pseudoscalar currents is given. Special attention is paid to the description of the large-$N_f$ results, obtained in collaboration with Broadhurst and Maxwell, for the scalar correlator, and estimates of its higher-order perturbative uncertainties within the renormalon-inspired large-$\beta_0$ expansion in the $\overline{\text{MS}}$ scheme are given. Brief discussion is presented of the results of calculations of higher-order perturbative QCD corrections to the relation between pole and $\overline{\text{MS}}$-scheme running-quark masses. Their comparison with the different estimates is also given.

Contributed to the Proceedings of Quarks-2000 International Seminar,
May 2000, Pushkin, Russia
Light-quark masses and renormalons

A.L. Kataev

Theoretical Physics Division, CERN CH-1211, Geneva, Switzerland
and Institute for Nuclear Research of the Academy of Sciences of Russia,
117312 Moscow, Russia

Abstract

A brief review of the problem of the determination of light-quark masses from QCD sum rules for the correlators of scalar and pseudoscalar currents is given. Special attention is paid to the description of the large-$N_f$ results, obtained in collaboration with Broadhurst and Maxwell, for the scalar correlator, and estimates of its higher-order perturbative uncertainties within the renormalon-inspired large-$\beta_0$ expansion in the $\overline{\text{MS}}$ scheme are given. Brief discussion is presented of the results of calculations of higher-order perturbative QCD corrections to the relation between pole and $\overline{\text{MS}}$-scheme running-quark masses. Their comparison with the different estimates is also given.

1 Introduction

The proposal to extract the values of light-quark current masses from the QCD sum rules for the correlators of quark scalar and pseudoscalar currents is rather old (see e.g. the works of Refs. [1]–[6] and the reviews of Refs. [7]–[9]). However, in view of the appearance of new experimental data and new theoretical results and ideas, the investigations in this direction are continuing (for a summary of the modern situation, see for instance the reviews of Refs. [10, 11]).

When studies began, it was not clear what normalization point should be associated with the definite values of the light-quark current masses. Starting from the mid-90s it became common wisdom, accepted by the Particle Data Group, to consider as phenomenological parameters the running quark masses of the $\overline{\text{MS}}$ scheme, normalized at either 1 GeV or 2 GeV. Another quantity, probably more suitable for the calculations on the lattice, is the renormalization-scheme-invariant mass $\hat{m}$, connected with the running one by the following solution of the renormalization group equation

$$m(Q^2) = \hat{m} \exp \left[ - \int_0^{\alpha_s(Q^2)} \frac{\gamma_m(x)}{\beta(x)} dx - \int_0^{2\beta_0} \frac{\gamma_0}{\beta_0 x} dx + 2 \frac{\gamma_0}{\beta_0} \ln(2\beta_0) \right]$$

where the perturbative QCD $\beta$-function and the mass-anomalous dimension function $\gamma_m$ are now known at the 4-loop approximations (see Ref. [12] and Refs. [13, 14] respectively) with the one-loop scheme-independent terms $\beta_0 = \frac{11 - (2/3)N_f}{4}$ and $\gamma_0 = 1$.

Another important definition of the current masses is the on-shell or pole quark masses. Despite the fact that, contrary to the case of charged leptons, quarks do not exist as free particles, this definition is commonly accepted and widely used when heavy quarks are considered.
Within perturbation theory and the $\overline{\text{MS}}$ scheme, the running quark masses and pole quark masses can be straightforwardly connected. At the next-to-leading order (NLO) this relation was calculated in Ref. [15] and confirmed later on in Ref. [16]. Beyond the NLO level, higher order terms to this relation were estimated in the large-$\beta_0$ approximation [17, 18], which can be obtained from the gauge-independent large-$N_f$ expansion after renormalon-inspired substitution $N_f \to -6\beta_0$. At the NNLO level the correction to the relation between pole and running quark masses was estimated in Ref. [19] within the framework of the scheme-invariant approach developed in the works of Ref. [20].

The results of the subsequent approximate NNLO calculations, made by evaluating expansions of the 3-loop quark self-energy for small and large external momentum and further Padé improvements of the corresponding mass-dependent series [21], turned out to be in reasonable agreement with estimates, obtained by both large-$\beta_0$ resummation [17, 18] and scheme-invariant methods [19]. In its turn, the numerical result of the approximate calculation of Ref. [21] was confirmed by the recent explicit analytical calculations, performed in Ref. [22].

In this report the survey of the uncertainties of recent QCD sum-rule determinations of light-quark masses from the correlators of scalar and pseudoscalar currents at 3-loop [23]–[25] and 4-loop [26] perturbative QCD approximations is given. Indeed, a single-chain renormalon structure of the Borel images of the functions, related to the correlator of scalar quark currents was recently studied in collaboration with Broadhurst and Maxwell in Ref. [28]. In this note special attention is paid to the results obtained in Ref. [28]. The higher-order perturbative QCD uncertainties for the studied functions are estimated with the help of the large-$\beta_0$ approximation. The bridge between the analysis of similar questions in the case of the relation between pole and running quark masses, which contain the renormalon singularity [29, 30], will also be constructed. The reason for the limitations of the scheme-invariant estimates of Ref. [13] in the scalar channel will be clarified.

## 2 Renormalon calculus

The studies of renormalon effects (for reviews see, [31, 32]) usually start from the consideration of the contributions of the internal single chain of fermion loops to some physical quantity $D$, say to the anomalous magnetic moment of the electron [33] or to the $e^+e^-$-annihilation Adler function [34, 35]. From a perturbative point of view, these insertions form the basis of the large-$N_f$ expansions, which are widely used at present. In principle, the coefficients of these expansions are scheme-dependent (for the discussion of the scheme dependence of renormalon contributions, see Ref. [36]), but in what follows this problem will not be analysed since the $\overline{\text{MS}}$ scheme will be essentially used.

The next step in the renormalon calculus is the construction, from a perturbative expansion of the physical quantity $D(a)$

$$D(a) = \sum_{n \geq 0} d_n a^{n+1}$$

(2)
of the Borel transform
\[ B[D](\delta) = \sum_{n \geq 0} d_n \delta^n / n! , \] (3)
and of the Borel integral
\[ \tilde{D}(a) = \int_0^\infty e^{-\delta/a} B[D](\delta) \, d\delta . \] (4)
The basic step in defining this integral is related to the analysis of the singularities of the Borel transform $B[D(\delta)]$. In the case when it has no singularities on the real positive axis $\delta$, the integral of Eq. (3) is well defined. The singularities, located on the negative axis $\delta$, are called ultraviolet (UV) renormalons; after Borel resummation, they generate the sign-alternating perturbative QCD series with factorially increasing coefficients. The singularities, located on the positive axis $\delta$ are called infrared (IR) renormalons. These are associated with the sign constant QCD perturbative expansions with coefficients, increasing like $n!$. In this case the Borel integral is ill-defined, but its Cauchy Principle Value (PV) can be used (for one of the first applications to the resummation of the renormalon-chain, perturbative contributions to the $(g - 2)/2$ of electron, in QED [33] with coefficients growing like $(+1)^n n!$, see Ref. [37]). In fact, it is possible to show that the IR renormalon singularities can be associated to power-suppressed corrections of order $(\Lambda/Q)^{(2p)}$, where $p$ is the number, related to the pole singularity, at the points $\delta$ of the positive axis of the Borel plane (see e.g. Ref. [32]).

Up to now all discussions were made within the framework of large-$N_f$ expansion, which is well-defined in the cases of both QED and QCD. It should be stressed that, since the first coefficient of the QED $\beta$-function is proportional to $N_f$, the large-$N_f$ limit of QED is identical to the large-$\beta_0$ approximation. In the case of QCD the situation is more ambiguous. Indeed, in order the rewrite the large-$N_f$ perturbative series in the form of the large-$\beta_0$ approximation the naive nonabelianization ansatz [38], namely the substitution $N_f \rightarrow N_f - 11N_c/2 = -6\beta_0$ should be used. This procedure turned out to be rather useful in the analysis of both renormalon effects and estimates of the uncertainties due to perturbative corrections beyond the calculated ones (see e.g. Ref. [39]).

3 Definitions of the basic quantities

Consider now the correlator of scalar quark currents $J_S = m(\mu) \bar{\psi}\psi$, namely the Green function
\[ \Pi_S(Q^2) = i \int e^{iqx} \langle J_S(x)J_S(0) \rangle_0 d^4x . \] (5)
Its imaginary part $\text{Im}\Pi_S = 2\pi sR_S (1 + O(1/s))$ is related to the spectral function $R_S(s)$ of two Euclidean constructs, considered in the work of Ref. [28]:
\[ \tilde{D}_S(Q^2) = Q^2 \int_0^\infty \frac{R_S(s)}{(s + Q^2)^2} \, ds \] (6)
\[ \overline{D}_S(Q^2) = 2Q^2 \int_0^\infty \frac{sR_S(s)}{(s + Q^2)^3} \, ds . \] (7)
The first one is defined through the dispersion relation for the first derivative of $\Pi_S(Q^2)/Q^2$, while the second one is defined by the second derivative for $\Pi_S(Q^2)$. The $\tilde{D}(Q^2)$-function was used in the process of calculating the 2-loop and 3-loop QCD corrections to $R_S(s)$ in the $\overline{\text{MS}}$ scheme in Refs. [40]-[42]. The 4-loop QCD logarithmic corrections to $\Pi_S$, and therefore the $\alpha_s^3$ contributions to its imaginary part $\tilde{R}_S(s)$, were evaluated in Ref. [43]. In the process of these calculations the following inhomogeneous renormalization group equation was used:

\[
\left( \frac{\partial}{\partial \log \mu^2} + \beta(\alpha_s) \frac{\partial}{\partial \alpha_s} + 2\gamma_m(\alpha_s) \right) \Pi_S = [m(\mu^2)]^2 Q^2 \left[ \gamma_{SS}(\alpha_s) + O\left( \frac{m^2}{Q^2} \right) \right] .
\] (8)

In leading order in $1/Q^2$, and next-to-leading order in $1/N_f$, we have [28]:

\[
\Pi_S = [m(\mu^2)]^2 Q^2 d_F \left( -2L - 4 + \frac{C_F b}{T_f N_f} H(L, b) + O\left( \frac{1}{N_f^2} \right) \right),
\] (9)

\[
\gamma_{SS} = d_F \left( -2 + \frac{C_F b}{T_f N_f} h(b) + O\left( \frac{1}{N_f^2} \right) \right),
\]

where $d_F = 3$, $C_F = 4/3$, $L = \ln(\mu^2/Q^2)$ and $b = T_f N_f \alpha_s/(3\pi)$. The expression of the coefficients $H_n(L)$ of the large-$N_f$ expansion of $H(L, b)$, namely $H(L, b) = \sum_{n>1} H_n(L) b^{n-2}$, can be obtained from the all-order solution of the following relation [28]:

\[
n(n-1)H_n(L) = n \left( h_{n+1} - 4(L+2)g_n \right) + 4g_{n+1} - 9(-1)^n D_n(L)
\] (10)

\[
\sum_n \frac{D_n(L) \delta^n}{n!} = \left[ 1 + \delta G_D(\delta) \right] \exp \left( \left( L + \frac{5}{3} \right) \delta \right),
\]

where $h_n$ are defined by the large-$N_f$ expansion of the $h(b)$-function in the expression for $\gamma_{SS}$:

\[
h(b) = \sum_{n \geq 1} \left( T_f N_f \frac{\alpha_s}{3\pi} \right)^{n-2} \left[ h_n + O\left( \frac{1}{N_f} \right) \right]
\] (11)

and $g_n$ are the numbers that are generated through the $\epsilon$-expansion of the following identity

\[
\sum_n g_n \epsilon^{n-1} = \left[ 4 - \sum_{n>1} \left( \frac{3}{2n} + \frac{n}{2} \right) \epsilon^{n-2} \right] \exp \left( \sum_{l>2} \frac{2l-3}{l} (-1)^l \zeta(l) \epsilon^l \right). \] (12)

### 4 Unravelling the $\delta = 1$ IR renormalon knot

The contributions of both UV and IR renormalons to $\Pi_S$ is given by the corresponding expression for $G(\delta)$ [28]:

\[
G_D(\delta) = \frac{2}{1-\delta} - \frac{1}{2-\delta} + \frac{8(1-\delta)}{3} \sum_{k=2}^{\infty} \frac{(-1)^k k}{(k^2 - (1-\delta)^2)^2}
\] (13)
It can be separated into two pieces as $G_D(\delta) = G_-(\delta) + G_+(\delta)$. The Borel resummable UV renormalons are contained in the first term

$$G_-(\delta) = -\frac{2}{3} \sum_{k>0} \frac{(-1)^k}{(k+\delta)} ,$$

(14)

with singularities located at $\delta < 0$. At the large-$N_f$, limit it generates the sign-constant asymptotic series. After performing a naive nonabelianization, namely after the replacement $b \rightarrow -\beta_0 \alpha_s(\mu^2)/\pi$, one obtains sign-alternating asymptotic perturbative QCD series for $\Pi_S$.

The IR renormalons are defined by $G_+(\delta)$, which has the following expression

$$G_+(\delta) = \frac{2}{1-\delta} - \frac{1}{2-\delta} + \frac{2}{3} \sum_{k>2} \frac{(-1)^k}{(k-\delta)^2} .$$

(15)

Contrary to the vector case (see e.g. Ref. [44]) one can observe the appearance in Eq. (15) of the first IR renormalon at $\delta = 1$. In accordance with the general rules of renormalon calculus, this IR renormalon generates the $\Lambda^2/Q^2$ contribution to the $\tilde{D}_S(Q^2)$-function of Eq. (6). It should be stressed that this term cannot appear within the operator-product expansion machinery. Indeed, the first higher-twist operator, contributing to the $\tilde{D}_S(Q^2)$-function in the massless scheme comes from the gluon condensate $\langle (\alpha_s/\pi)G_2^2 \rangle_0$ [45], related to the IR renormalon pole at $\delta = 2$ (note that the perturbative QCD correction to the gluon condensate was calculated in Ref. [46]).

The reason for the appearance of the $\delta = 1$ IR renormalon contribution to the $\tilde{D}_S$-function is related to the fact that the dispersion relation of Eq. (6) is ill-defined. Indeed, contrary to the vector case, where the Ward identity allows us to fix the expression for $\Pi_V(Q^2)$ at zero transferred momentum, the expression for $\Pi_S(0)$ is infinite. Therefore, the dispersion relation for the first derivative of $\Pi_S(Q^2)/Q^2$ of Eq. (6) contains an ambiguity of order $\Lambda^2/Q^2$. For large momentum transfer this problem can be neglected. However, one should avoid the application of Eq. (6) in the process of long-distance studies, e.g. the determination of light-quark masses values. In this case it is necessary to use the dispersion relation for the second derivative of $\Pi_S$ (see Eq. (7)), which is free from unphysical $\Lambda^2/Q^2$ term. This renormalon rediscovery of the advantages of the twice-differentiated Euclidean construct of Eq. (7), which was originally used in Ref. [4] and later on in Refs. [24]–[27], is setting its application for the extraction of light-quark masses on a more solid background. It should also be mentioned, that the spectral density $R_S(s)$ of both Eq. (6) and Eq. (7) is also free from contributions of $\delta = 1$ IR renormalon. Moreover, since the factor $\pi \delta/\sin(\pi \delta)$ of analytic continuation of the Euclidean constructs to the Minkowskian region is removing all single poles in Eq. (15) and transforming double poles in $\delta$ into single poles, the Borel image of $R_S(s)$ contains $\delta > 2$ IR renormalons only, which are associated with the contributions to $R_S(s)$ of the operators $O_k$ with dimension $d_k \geq 6$. 
5 Correlator of scalar quark currents and large-\(\beta_0\) expansion

The large-\(\beta_0\) expansion in the \(\overline{\text{MS}}\) scheme is widely used to generate perturbative series from the direct calculations of the renormalon-chain diagrams, which contain the information on both UV and IR renormalons structure of the related Borel transforms. Let us summarize the results of its application for modelling the behaviour of the perturbative expansions for basic quantities, related to the correlators of the scalar and pseudoscalar quark currents (see Ref. [28]). The quantities defined above in Eqs. (6),(7) have the following expansions:

\[
\begin{align*}
\tilde{D}_S(Q^2) &= 3[m(Q^2)]^2 \left(1 + \sum_{n>0} d_n a^n\right) \quad (16) \\
\overline{D}_S(Q^2) &= 3[m(Q^2)]^2 \left(1 + \sum_{n>0} \tilde{d}_n a^n\right) \quad (17) \\
R_S(s) &= 3[m(s)]^2 \left(1 + \sum_{n>0} s_n a^n\right) \quad (18)
\end{align*}
\]

In leading order of the large-\(\beta_0\) expansion, the coefficients of these series, obtained using the naive nonabelianization procedure, can be presented as

\[
\begin{align*}
d^{\text{NNA}}_n &= \beta_0^{n-1} \tilde{\Delta}_{n+1} \quad (19) \\
s^{\text{NNA}}_n &= \beta_0^{n-1} \Delta_{n+1} \quad (20) \\
\tilde{d}^{\text{NNA}}_n &= \beta_0^{n-1} \overline{\Delta}_{n+1} \quad (21)
\end{align*}
\]

where the coefficients \(\tilde{\Delta}_{n+1}\), \(\Delta_{n+1}\) and \(\overline{\Delta}_{n+1}\) were calculated in Ref. [28] in the \(\overline{\text{MS}}\) scheme. The concrete results of calculations are presented in Table 1.

**Table 1:** The values of coefficients in Eqs. (19),(20),(21).

| \(n\) | \(\Delta_n\) | \(\Delta_{n+1}\) | \(\overline{\Delta}_n\) |
|-------|----------------|-----------------|-----------------|
| 2     | 7.33333        | 7.33333         | 5.33333         |
| 3     | 10.4696        | 7.17968         | 3.13622         |
| 4     | 32.6145        | 8.48885         | 11.6754         |
| 5     | 97.9534        | 4.36402         | 0.10978         |
| 6     | 503.887        | 2.96849         | 112.074         |
| 7     | 2194.28        | -54.2101        | -325.157        |
| 8     | 16465.8        | 123.639         | 3300.11         |

One can see that the coefficients \(\tilde{\Delta}_{n+1}\) are increasing very fast. This feature is related to the manifestation of \(\delta = 1\) IR renormalon contribution to Eq. (13). The suppression of this singularity in the expressions for \(R_S(s)\) and \(\overline{D}_S(Q^2)\) leads to a rather well-behaved perturbative series up to \(n = 6\)-loop order for \(R_S(s)\) and \(n = 5\)-loop order in the latter case, where the
corresponding coefficient $\Delta_5$ is remarkably small. The factorial growth of the related series starts to manifest itself at the level of higher-order corrections.

Consider now the uncertainties of the large-$\beta_0$ series, comparing the numerical values for the coefficients of Eqs. (19), (20), (21) with the explicit numbers, obtained as the result of analytical calculations, performed in Refs. [40]–[43] (see Table 2).

Table 2: Ratios of NNA estimates to exact results.

| Coef. | $N_f = 3$ | $N_f = 4$ | $N_f = 5$ |
|-------|-----------|-----------|-----------|
| $d^\text{NNA}_2 / d_2$ | 0.514 | 0.496 | 0.477 |
| $s^\text{NNA}_2 / s_2$ | 0.507 | 0.490 | 0.472 |
| $\overline{d}^\text{NNA}_2 / \overline{d}_2$ | 0.498 | 0.484 | 0.469 |
| $d^\text{NNA}_3 / d_3$ | 0.354 | 0.346 | 0.339 |
| $s^\text{NNA}_3 / s_3$ | 0.482 | 0.565 | 0.747 |
| $\overline{d}^\text{NNA}_3 / \overline{d}_3$ | 0.764 | 0.871 | 1.081 |

One can see that contrary to the applications of the scheme-invariant approach for estimates of higher-order perturbative QCD corrections in the scalar channel [19], the large-$\beta_0$ approximation gives the correct signs for the coefficients of all considered quantities. The reason for the failure of the scheme-invariant estimates at the 4-loop level will be clarified below. It should also be stressed that although the large-$\beta_0$ predictions are of the same order of magnitude as the exactly calculable coefficients, the application of the naive nonabelianization procedure in the scalar channel has the tendency to underestimate the concrete perturbative terms by a factor of order 0.5. Keeping this in mind, and taking into account the results from Table 1, we arrive at the conclusion that the large-$\beta_0$ approximation indicates, that the 5-loop corrections to the perturbative series for the $\overline{D}_S$ function and $R_S(s)$, which enter in the determination of the strange-quark mass within QCD sum rules method (see Refs. [2],[24]–[27]), are extremely small. Indeed, fixing $N_f = 3$ and $\alpha_s \approx 0.3$ we obtain

\[
\overline{D}_S = 1 + 3.67 \left( \frac{\alpha_s}{\pi} \right) + 14.17 \left( \frac{\alpha_s}{\pi} \right)^2 + 77.36 \left( \frac{\alpha_s}{\pi} \right)^3 + 2 \times 1.26 \left( \frac{\alpha_s}{\pi} \right)^4 \quad (22)
\]

and

\[
R_S(s) = 1 + 5.667 \left( \frac{\alpha_s}{\pi} \right) + 31.864 \left( \frac{\alpha_s}{\pi} \right)^2 + 89.156 \left( \frac{\alpha_s}{\pi} \right)^3 + 98 \left( \frac{\alpha_s}{\pi} \right)^4 \quad (23)
\]

Therefore, large-$\beta_0$ estimates indicate that the doubts about a serious underestimate of the errors of the QCD strange-quark-mass extraction from the pseudoscalar correlator at the ($\alpha_s^2$)-order [24], formulated in Ref. [17] using the positivity of a spectral function for a pseudoscalar correlator, cannot be related to the non-applicability of the perturbative QCD expansions at rather small energy scale. Moreover, the $O(\alpha_s^3)$ result of Ref. [20] $\overline{m}_s(1 \text{ GeV}) = 205 \pm 19$ MeV is closer to the upper bound from Ref. [17], namely $140 \leq \overline{m}_s(1 \text{ GeV}) \leq 254$ MeV. At the energy
scale of 2 GeV the results of Ref. [26] are equivalent to the value $m_s(2 \text{ GeV}) \sim 148 \text{ MeV}$, which are higher than the current lattice results (for a review, see Ref. [11]). Note, however, that the current determination of light-quark masses from QCD sum rules for the scalar and pseudoscalar two-point functions does not touch the problem of the possible manifestation of the instanton contributions in the theoretical part of these sum rules (see Ref. [15]). This is why the determination of the $s$-quark mass in Cabibbo-suppressed $\tau$-lepton decay characteristics, which seem to be free from instanton contributions, attracts more and more attention (see e.g. Ref. [49] and in particular Ref. [50]). Note that the central value of the $s$-quark mass result of Ref. [50], namely $m_s(1 \text{ GeV}) = 176 \pm 37_{\exp} \pm 13_{\text{th}} \text{ MeV}$, which is equivalent to $m_s(2 \text{ GeV}) \sim 128 \text{ MeV}$, is lower than of the one of Ref. [26] and is closer to the lattice results, summarized in the review of Ref. [11]. One of the reasons can be related to the approach applied in Ref. [50], of resummation of the infinite subset of $\pi^2$-dependent effects that arise from analytical continuation of the mass-dependent quantities from the Euclidean to the Minkowskian region. Within the large-$\beta_0$ approximation the special features of this procedure were studied in Ref. [28].

6 Pole vs running quark masses and the large-$\beta_0$ approximation

Another example where the naive nonabelianization procedure [38] and the large-$\beta_0$ estimates are working reasonably well, is the relation between pole and running quark masses. Indeed, this relation was recently evaluated analytically at the $\alpha_s^3$-order [22]. The results of these calculations, which confirm those obtained in Ref. [21] in a semi-analytical way, have the following numerical form [22]:

$$M = \overline{m}(\overline{m}) \left[ 1 + \frac{4}{3} \left( \frac{\overline{\pi}_s}{\pi} \right) + \left( \frac{\overline{\pi}_s}{\pi} \right)^2 \left( -1.0414N_f + 13.4434 \right) \right. $$

$$ + \left. \left( \frac{\overline{\pi}_s}{\pi} \right)^3 \left( 0.6527N_f^2 - 26.655N_f + 190.595 \right) \right] $$

with $\overline{\alpha}_s = \overline{\alpha}_s(\overline{m})$. This series can be rewritten in terms of the scheme-independent coefficients of the QCD $\beta$-function as [22]:

$$M = \overline{m}(\overline{m}) \left[ 1 + \frac{4}{3} \left( \frac{\overline{\pi}_s}{\pi} \right) + \left( \frac{\overline{\pi}_s}{\pi} \right)^2 \left( 6.248\beta_0 - 3.739 \right) \right. $$

$$ + \left. \left( \frac{\overline{\pi}_s}{\pi} \right)^3 \left( 23.497\beta_0^2 + 6.248\beta_1 + 1.019\beta_0 - 29.94 \right) \right] ,$$

where $\beta_0$ is as defined above and $\beta_1 = [102 - (38/3)N_f]/16$. It is possible now to deduce that the large-$\beta_0$ approximation works reasonably well in this case as well, thanks to the cancellations between the term proportional to the $\beta_1$ coefficient and the conformal $\beta$-independent one, in the order correction of order $\alpha_s^3$ to Eq. [23] the large-$\beta_0$ approximation is working reasonably well ![1]. This feature is also illustrated in Table 3, taken from Ref. [21], where the comparison

---

[1] I wish to thank E. Gardi for discussions on questions related to this topic.
of the results of semi-analytic calculations of the $O(\alpha_s^3)$ correction to Eq. (24) [21], presented in the second column, are compared with the estimates of these terms, made in Ref. [19] using the scheme-invariant methods (namely the effective-charges approach (ECH) of Ref. [51] and the PMS approach of Ref. [52]) and the large-$\beta_0$ estimates of Ref. [17].

Table 3: Comparison of the results of Ref. [21] paper with estimates based on ECH, PMS and the large-$\beta_0$ approximation for $M/\overline{m}(\bar{m})$.

| $N_f$ | $[21]$ | [19] (ECH) | [19] (PMS) | [17] (large-$\beta_0$) |
|-------|--------|------------|------------|------------------------|
| 2     | 143(3) | 152.71     | 153.76     | 137.23                 |
| 3     | 119(3) | 124.10     | 124.89     | 118.95                 |
| 4     | 96(2)  | 97.729     | 98.259     | 101.98                 |
| 5     | 75(2)  | 73.616     | 73.903     | 86.318                 |

One can see that the scheme-invariant methods, developed in other cases in Ref. [20], also give reasonable estimates. However, there are cases, where the comparison of the results of estimates, produced by scheme-invariant methods or the large $\beta_0$-approach, with the explicitly calculated corrections of the perturbative series under consideration, demonstrate larger ambiguities.

7 Limitations of estimating procedures: when and why?

It should be mentioned that unlike the case of the qualitative success of the large-$\beta_0$ estimates in Ref. [28] of the coefficients of the perturbative series of quantities related to the Green function of the scalar and pseudoscalar quark currents, the application of the scheme-invariant estimates in this case result in the appearance of large and negative order $\alpha_s^4$ corrections in the expression for $R_S(s)$ [19]. It is thus worth-while trying to understand the reason for the appearance of these suspicious numbers and, therefore, the limitations of the applications of the scheme-invariant procedure of Ref. [20], used in Ref. [19]. These studies were done in Ref. [28] and their main conclusions will be summarized here.

It is worth-while recalling that the approach of Ref. [20] is constructed for the estimates of higher-order perturbative corrections to renormalization-group-invariant quantities of Eq. (2), which obey the renormalization-group equation without anomalous dimension term, with the $\beta$-function defined as $\beta(a) = -\sum_{i \geq 0} \beta_i a^{i+2} = -\beta_0 a^2 (1 + \sum_{i \geq 1} c_i a^i)$, where $c_i = \beta_i / \beta_0$. It is known that the method of the effective charges of Ref. [51] prescribes to define the scheme where all higher-order corrections to $D(a)$ will be nullified and the corresponding expression will have the following form: $D(\tilde{a}) = d_0 \tilde{a}$. The new expansion parameter obeys the renormalization-group equation with the effective-charges $\beta$-function, defined as

$$\tilde{\beta}(\tilde{a}) = -\sum_{n \geq 0} \tilde{\beta}_n \tilde{a}^{n+2},$$

(26)
where the coefficients $\tilde{\beta}_n$ are scheme-invariant. The basic formula for generating the estimates from the scheme-invariant procedure of Ref. [20] is:

$$\frac{\tilde{\beta}_n - \beta_n}{(n-1)} = \beta_0(d_n - \Omega_n) \ ,$$  \hspace{1cm} \text{(27)}

where $\Omega_n$ are defined as

$$\begin{align*}
\Omega_2 &= d_1(c_1 + d_1) \hspace{1cm} \text{(28)} \\
\Omega_3 &= d_1\left(c_2 - \frac{1}{2}c_1d_1 - 2d_1^2 + 3d_2\right) \\
\Omega_4 &= d_1\left(c_3 - \frac{4}{3}c_2d_1 + \frac{2}{3}c_1d_2 + \frac{14}{3}d_1^3 - \frac{28}{3}d_1d_2 + 4d_3\right) \\
&\quad + \frac{1}{3}\left(c_2d_2 - c_1d_3 + 5d_2^2\right) \hspace{1cm} \text{(29)}
\end{align*}$$

at 5 loops. The idea that lies beyond the procedure of Ref. [20] is that reasonable estimates of the higher-order coefficients $d_n$ of the perturbative series for physical quantities can be obtained if the coefficients $\tilde{\beta}_n$ of the process-dependent, effective-charges $\beta$-functions are of the same sign and magnitude as the coefficients $\beta_n$ of the $\beta$-function in the $\overline{\text{MS}}$ scheme. This assumption turns out to be true at the 4-loop level in QCD for the perturbative series of deep-inelastic scattering sum rules and the $e^+e^-$-annihilation $D$-function, in the cases $N_f = 4$ and $N_f = 3$ in particular. Indeed the numerical analogues of the analytical expressions for the 4-loop QCD $\beta$-function [12] have the following form

$$\begin{align*}
\beta(N_f = 3) &= -2.250a^2 - 4.000a^3 - 10.600a^4 - 47.228a^5 \hspace{1cm} \text{(30)} \\
\beta(N_f = 4) &= -2.083a^2 - 3.208a^3 - 6.349a^4 - 31.387a^5 \hspace{1cm} \text{(31)} \\
\beta(N_f = 5) &= -1.917a^2 - 2.417a^3 - 2.827a^4 - 18.852a^5 \hspace{1cm} \text{(32)}
\end{align*}$$

with $a \equiv \alpha_s/\pi$. It should be stressed that at $N_f = 3$ and $N_f = 4$ the effective-charges $\beta$-functions of the polarized and unpolarized Bjorken sum rules and of the $e^+e^-$-annihilation $D$-function have a similar 4-loop behaviour, provided the explicitly unknown coefficients $d_3$ in $\Omega_4$ are modelled by the numerical expressions for $\Omega_3$. However, this is not true in the case of renormalization-group-invariant quantities, related to the correlators of scalar and pseudoscalar currents. Indeed, for the renormalization-group-invariant quantity related to the $\overline{D_s}$-function of Eq. (7) as

$$\overline{R}_D(Q^2) = -\frac{1}{2} \frac{d\log\overline{D}_s(Q^2)}{d\log Q^2} \hspace{1cm} \text{(33)}$$

the behaviour of the effective-charges $\beta$-function in the $O(\tilde{a}^3)$ and $O(\tilde{a}^3)$-approximations differs significantly from the behaviour of Eqs. (30),(31),(32) [28]. The corresponding expressions

$$\begin{align*}
\tilde{\beta}(N_f = 3) &= -2.250\tilde{a}^2 - 4.000\tilde{a}^3 + 58.920\tilde{a}^4 - 2148.503\tilde{a}^5 \\
\tilde{\beta}(N_f = 4) &= -2.083\tilde{a}^2 - 3.208\tilde{a}^3 + 53.852\tilde{a}^4 - 1687.191\tilde{a}^5 \\
\tilde{\beta}(N_f = 5) &= -1.917\tilde{a}^2 - 2.417\tilde{a}^3 + 49.356\tilde{a}^4 - 1303.490\tilde{a}^5
\end{align*}$$

\hspace{1cm} \text{(34)-(36)}
indicate the appearance of a spurious perturbative infrared fixed point. This spurious zero
is compensated by the appearance of large and negative $\tilde{a}^5$ contributions. In the case of the
$R_D$-function, similar features were already observed at the 3-loop level in Ref. [12] and at the
4-loop in Ref. [13] both in the Minkowskian region; they were studied in detail in the Euclidean
region in Ref. [54]. Here we conclude that these features demonstrate the limitations of the
application of the scheme-invariant methods to the estimates of the $O(\alpha_s^4)$-corrections to the
$D_S$ function of Eq. (6), the $\overline{D}_S$ function of Eq. (7), and their spectral density $R_S(s)$.

However, the approximation of the large $\beta_0$-expansion, which we think is working reason-
ably well in the case of the correlator of the scalar and pseudoscalar quark currents [28], also
has definite limitations. The inapplicability of this method for the estimates of higher-order
corrections to the DGLAP non-singlet kernel, studied in detail in Ref. [54], can be explained by
the absence of renormalon-type contributions to the anomalous dimensions of the non-singlet
operators. A more interesting fact is related to the contradiction between the large-$\beta_0$ estimates
of the high-order perturbative corrections to the coefficient functions of $N = 2$ and $N = 4$ non-
singlet Mellin moments, for the $F_2$ structure function [55], and the result of explicit calculations
performed in Ref. [56]. The limitations of the predictive possibilities of the large-$\beta_0$ method in
this case are still unclear.

Acknowledgements

I am grateful to D.J. Broadhurst and C.J. Maxwell for the productive and pleasant col-
laboration, which resulted in the publication of Ref. [28]. Different aspects of this work were
discussed at the Quarks-2000 International Seminar in the talks of D.J.B. and A.L.K., and
are described in part above. It is a pleasure to thank G. Altarelli, V.M. Braun, J. Ellis, J.
Fischer, N.V. Krasnikov, S.A. Larin, N. Paver, A.A. Pivovarov, A. Schafer and F.J. Yndurain
for discussions and constructive questions and comments.

Part of the work on the problems approached in this paper was done in Russia within the
framework of scientific projects of RFBR Grants N 99-01-00091, N 00-02-1742.

References

[1] A. I. Vainshtein, M. B. Voloshin, V. I. Zakharov, V. A. Novikov, L. B. Okun and M. A. Shif-
man, Sov. J. Nucl. Phys. 27 (1978) 274.
[2] C. Becchi, S. Narison, E. de Rafael and F. J. Yndurain, Z. Phys. C8, 335 (1981).
[3] A. L. Kataev, N. V. Krasnikov and A. A. Pivovarov, Phys. Lett. B123 (1983) 93.
[4] S. Narison, N. Paver, E. de Rafael and D. Treleani, Nucl. Phys. B 212 (1983) 365.
[5] S. G. Gorishny, A. L. Kataev and S. A. Larin, Phys. Lett. B135 (1984) 457.
[6] C. A. Dominguez and E. de Rafael, Ann. Phys. 174 (1987) 372.
[7] J. Gasser and H. Leutwyler, Phys. Rep. 87 (1982) 77.

[8] A. L. Kataev, N. V. Krasnikov and A. A. Pivovarov, Preprint INR-P-0389 (1984); 
in Proc. Quarks-84 Int. Seminar, Tbilisi, 1984.

[9] S. Narison, Riv. Nuovo Cim. 10 (1987) 1.

[10] S. Narison, Nucl. Phys. Proc. Suppl. 86 (2000) 242 [hep-ph/9911454].

[11] R. Gupta and K. Maltman, hep-ph/0101132.

[12] T. van Ritbergen, J. A. Vermaseren and S. A. Larin, Phys. Lett. B400 (1997) 379 [hep-
ph/9701390].

[13] K. G. Chetyrkin, Phys. Lett. B404 (1997) 161 [hep-ph/9703278].

[14] J. A. Vermaseren, S. A. Larin and T. van Ritbergen, Phys. Lett. B405 (1997) 327 [hep-
ph/9703284].

[15] N. Gray, D. J. Broadhurst, W. Grafe and K. Schilcher, Z. Phys. C48 (1990) 673.

[16] J. Fleischer, F. Jegerlehner, O. V. Tarasov and O. L. Veretin, Nucl. Phys. B539 (1999) 
671 [hep-ph/9803493].

[17] M. Beneke and V. M. Braun, Phys. Lett. B348 (1995) 513 [hep-ph/9411229];

P. Ball, M. Beneke and V. M. Braun, Nucl. Phys. B452 (1995) 563 [hep-ph/9502300].

[18] K. Philippides and A. Sirlin, Nucl. Phys. B450 (1995) 3 [hep-ph/9503434].

[19] K. G. Chetyrkin, B. A. Kniehl and A. Sirlin, Phys. Lett. B402 (1997) 359 [hep-
ph/9703226].

[20] A. L. Kataev and V. V. Starshenko, Mod. Phys. Lett. A10 (1995) 235 [hep-ph/9502348].

A. L. Kataev and V. V. Starshenko, Phys. Rev. D 52 (1995) 402 [hep-ph/9412305].

[21] K. G. Chetyrkin and M. Steinhauser, Phys. Rev. Lett. 83 (1999) 4001 [hep-ph/9907509].

[22] K. Melnikov and T. v. Ritbergen, Phys. Lett. B482 (2000) 99 [hep-ph/9912391].

[23] J. Bijnens, J. Prades and E. de Rafael, Phys. Lett. B348 (1995) 226 [hep-ph/9411283].

[24] K. G. Chetyrkin, C. A. Dominguez, D. Pirjol and K. Schilcher, Phys. Rev. D 51 (1995) 
5090 [hep-ph/9409374].

[25] M. Jamin and M. Munz, Z. Phys. C66 (1995) 633 [hep-ph/9409333].

[26] K. G. Chetyrkin, D. Pirjol and K. Schilcher, Phys. Lett. B404 (1997) 337 [hep-
ph/9612394].

[27] P. Colangelo, F. De Fazio, G. Nardulli and N. Paver, Phys. Lett. B 408 (1997) 340 [hep-
ph/9704249].
[28] D. J. Broadhurst, A. L. Kataev and C. J. Maxwell, Nucl. Phys. B592 (2001) 247 [hep-ph/0007152].

[29] I. I. Bigi, M. A. Shifman, N. G. Uraltsev and A. I. Vainshtein, Phys. Rev. D 50 (1994) 2234 [hep-ph/9402360].

[30] M. Beneke and V. M. Braun, Nucl. Phys. B426 (1994) 301 [hep-ph/9402364].

[31] G. Altarelli, CERN-TH/95-309; in Proceedings of Int. School of Subnuclear Physics, July 1995, Erice, Italy.

[32] M. Beneke, Phys. Rep. 317 (1999) 1 [hep-ph/9807443];
M. Beneke and V. M. Braun, [hep-ph/0010208].

[33] B. Lautrup, Phys. Lett. B69 (1977) 109.

[34] V. I. Zakharov, Nucl. Phys. B385 (1992) 452.

[35] L. S. Brown, L. G. Yaffe and C. Zhai, Phys. Rev. D 46 (1992) 4712 [hep-ph/9205213].

[36] N. V. Krasnikov and A. A. Pivovarov, Mod. Phys. Lett. A11 (1996) 835 [hep-ph/9602272].

[37] A. S. Ilchev and V. K. Mitrjushkin, J. Phys. G G7 (1981) L221.

[38] D. J. Broadhurst and A. G. Grozin, Phys. Rev. D 52 (1995) 4082 [hep-ph/9410240].

[39] C. N. Lovett-Turner and C. J. Maxwell, Nucl. Phys. B452 (1995) 188 [hep-ph/9505224].

[40] S. G. Gorishny, A. L. Kataev and S. A. Larin, Sov. J. Nucl. Phys. 40 (1984) 329.

[41] S. G. Gorishny, A. L. Kataev, S. A. Larin and L. R. Surguladze, Mod. Phys. Lett. A5 (1990) 2703.

[42] S. G. Gorishny, A. L. Kataev, S. A. Larin and L. R. Surguladze, Phys. Rev. D 43 (1991) 1633.

[43] K. G. Chetyrkin, Phys. Lett. B390 (1997) 309 [hep-ph/9608318].

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

[45] M. A. Shifman, A. I. Vainshtein and V. I. Zakharov, Nucl. Phys. B147 (1979) 385.

[46] L. R. Surguladze and F. V. Tkachov, Nucl. Phys. B331 (1990) 35.

[47] F. J. Yndurain, Nucl. Phys. B517 (1998) 324 [hep-ph/9708300].

[48] E. Gabrielli and P. Nason, Phys. Lett. B313 (1993) 430.

[49] K. G. Chetyrkin, J. H. Kuhn and A. A. Pivovar, Nucl. Phys. B533 (1998) 473 [hep-ph/9805335].
[50] J. G. Korner, F. Krajewski and A. A. Pivovarov, `hep-ph/0003165`.

[51] G. Grunberg, Phys. Rev. D 29 (1984) 2315.

[52] P. M. Stevenson, Phys. Rev. D 23 (1981) 2916.

[53] E. Gardi and M. Karliner, Nucl. Phys. B 529 (1998) 383 `hep-ph/9802218`.

[54] S. V. Mikhailov, Phys. Lett. B 431 (1998) 387 `hep-ph/9804263`.

[55] L. Mankiewicz, M. Maul and E. Stein, Phys. Lett. B 404 (1997) 345 `hep-ph/9703356`.

[56] S. A. Larin, T. van Ritbergen and J. A. Vermaseren, Nucl. Phys. B 427 (1994) 41.