Contour-improved versus fixed-order perturbation theory in hadronic $\tau$ decays

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ABSTRACT: The hadronic decay rate of the $\tau$ lepton serves as one of the most precise determinations of the QCD coupling $\alpha_s$. The dominant theoretical source of uncertainty at present resides in the seeming disparity of two approaches to improving the perturbative expansion with the help of the renormalisation group, namely fixed-order and contour-improved perturbation theory. In this work it is demonstrated that in fact both approaches yield compatible results. However, the fixed-order series is found to oscillate around the contour-improved result with an oscillation frequency of approximately six perturbative orders, approaching it until about the 30th order, after which the expansion reveals its asymptotic nature. Additionally, the renormalisation scale and scheme dependencies of the perturbative series for the $\tau$ hadronic width are investigated in detail.

KEYWORDS: Hadronic $\tau$ decays, QCD coupling, summation of perturbation theory.
1. Introduction

Already more than a decade ago it was realised that the hadronic decay of the τ lepton could serve as an ideal system to study low-energy QCD under rather clean conditions [1–4]. In the following years, detailed investigations of the τ hadronic width as well as invariant mass distributions have served to determine the QCD coupling \( \alpha_s \) to a precision competitive with the current world average [5–10]. The experimental separation of the Cabibbo-allowed decays and Cabibbo-suppressed modes into strange particles [5, 11, 12] opened a means to also determine the quark-mixing matrix element \(|V_{us}|\) [13–15] as well as the mass of the strange quark [16–23], additional fundamental parameters within the Standard Model.

The starting point for a QCD analysis of the τ hadronic width \( R_\tau \) is the finite energy sum rule (FESR) [1, 24]

\[
\frac{\Gamma(\tau \to \text{hadrons } \nu_\tau)}{\Gamma(\tau \to \mu \bar{\nu}_\mu \nu_\tau)} \equiv R_\tau^{\Pi}(s_0) = \int_0^{s_0} w_\tau(s) \rho_\tau(s) \, ds = \frac{-1}{2\pi i} \oint_{|s|=s_0} w_\tau(s) \, \Pi_\tau(s) \, ds. \quad (1.1)
\]

The FESR can easily be derived from Cauchy’s theorem and the fact that the exact, non-perturbative correlation function \( \Pi_\tau(s) \) is analytic in the whole complex \( s \)-plane, except for the positive real axis, where it may have poles and cuts. The correlator \( \Pi_\tau(s) \) of hadronic QCD currents receives contributions from vector and axialvector correlation functions for both \((ud)\) as well as \((us)\) flavour content, dressed with the appropriate quark mixing matrix factors:

\[
\Pi_\tau(s) = |V_{ud}|^2 \left[ \Pi_{ud}^V(s) + \Pi_{ud}^A(s) \right] + |V_{us}|^2 \left[ \Pi_{us}^V(s) + \Pi_{us}^A(s) \right]. \quad (1.2)
\]
Furthermore, $\rho_\tau(s) \equiv \text{Im} \Pi_\tau(s + i0)/\pi$ is the so-called spectral function which contains all the physical information.

In the case of hadronic $\tau$ decays, $s$ is the invariant mass of the final hadron system, $w_\tau(s)$ is the relevant kinematic weight function,

$$w_\tau(s) = \frac{12\pi^2}{s_0} \left(1 - \frac{s}{s_0}\right)^2 \left(1 + 2 \frac{s}{s_0}\right), \quad (1.3)$$

and $s_0 = M_{\tau}^2$, though for the moment the somewhat more general expression will be kept. The fortuitous fact about $R_\tau$ is that the weight function introduces a double zero at $s = s_0$, such that there is no need to evaluate $\Pi_\tau(s)$ close to the real axis where perturbation theory becomes problematic. In writing eq. (1.1), a small contribution from longitudinal correlators has been omitted. Being suppressed by the light quark masses, it is of no relevance for the purpose of this work which will concentrate on the massless correlators, but it will be reconsidered in a subsequent publication.

Since the hadronic $\tau$ decay rate is a physical, measurable quantity, the corresponding perturbative QCD expression can be improved with the help of the renormalisation group equation (RGE). In the course of calculating $R_\tau \Pi_\tau(s_0)$, one also has to perform the contour integration over the circle with radius $s_0$ in the complex $s$-plane. Then the question arises in which order both operations should be performed. First calculating the contour integral and then performing the renormalisation group improvement goes under the name of fixed-order perturbation theory (FOPT) whereas the second approach of first resumming the expansion and afterwards integrating over the contour has been suggested in [25,26] and is termed contour-improved perturbation theory (CIPT). Both approaches will be investigated in much detail below.

Numerically, it is found that the CI perturbative expansion displays a better behaviour than the corresponding FO series [26]. In particular, employing the known perturbative results up to order $\alpha_s^3$ as well as estimates for the contributions at order $\alpha_s^4$ and $\alpha_s^5$, it is found that the difference between the two approaches is much larger than would be naively expected, based on the last included terms in the expansion. In the past, this apparent ambiguity has cast doubts as to which way of resumming the perturbative series is preferable and it represents the dominant source of theoretical uncertainty in the determination of $\alpha_s$ from the hadronic $\tau$ decay rate up to this day.

Below, it is demonstrated that in fact both approaches to the renormalisation group improvement of the perturbative series yield compatible results. However, the fixed-order series is found to oscillate around the contour-improved result with an oscillation frequency of approximately six perturbative orders, approaching it until about the 30th order, after which the expansion reveals its asymptotic nature. To this end, in the next section, the perturbative expansion of the vector correlation function will be reviewed, and in section 3 the two approaches of improving the perturbative series in the $\tau$-decay finite energy sum rule will be discussed. In section 4, a simplified example will be analysed, in which only the first coefficient of the $\beta$-function $\beta_1$ is non-vanishing. Whereas this case can be treated fully analytically, it shares all the essential features of the complete QCD expression. The more realistic case which includes all currently known terms in the $\beta$-function is then treated in
section 5. In section 6 and 7, the influence of variations of the renormalisation scale as well as the renormalisation scheme on the hadronic \( \tau \) decay rate are investigated, and, finally, in the conclusions my main findings of this work will be summarised.

2. Perturbative correlator

By far the most important contribution to the hadronic \( \tau \) decay rate is due to the purely perturbative vector (axialvector) correlation function in the limit of vanishing quark masses [1]. In this limit vector and axialvector correlators yield identical contributions. Therefore, in what follows, only the vector contribution will be investigated. A discussion of quark mass corrections shall be presented in a forthcoming publication, but for the remainder of this work, the quark masses are assumed to be zero.

In the massless case, the perturbative expansion of the vector correlation function \( \Pi(s) \) exhibits the general structure:\(^4\)

\[
\Pi(s) = -\frac{N_c}{12\pi^2} \sum_{n=0}^{\infty} a_\mu^n \sum_{k=0}^{n+1} c_{nk} L^k \quad \text{where} \quad L \equiv \ln \frac{-s}{\mu^2}, \tag{2.1}
\]

and \( a_\mu \equiv \alpha_s(\mu^2)/\pi \) with \( \mu \) being the renormalisation scale. (The global minus sign has been introduced for later convenience.) \( \Pi(s) \) itself is not a physical quantity. However, this is the case for the spectral function \( \rho(s) \) as well as for the Adler function \( D(s) \):

\[
D(s) \equiv -s \frac{d}{ds} \Pi(s) = \frac{N_c}{12\pi^2} \sum_{n=0}^{\infty} a_\mu^n \sum_{k=1}^{n+1} k c_{nk} L^{k-1}. \tag{2.2}
\]

It should be clear that the coefficients \( c_{n0} \) do not contribute to both the spectral function (because they are real) and to the Adler function (because of the factor \( k \)). Thus the coefficients \( c_{n0} \), which actually are found to depend on the renormalisation prescription, can be considered as “unphysical” in that they do not appear in measurable quantities.

As physical quantities, both \( D(s) \) as well as \( \rho(s) \) have to satisfy a homogeneous RGE:

\[
-\mu \frac{d}{d\mu} \begin{bmatrix} D(s) \\ \rho(s) \end{bmatrix} = \begin{bmatrix} 2 \frac{\partial}{\partial L} + \beta(a) \frac{\partial}{\partial a} \end{bmatrix} \begin{bmatrix} D(s) \\ \rho(s) \end{bmatrix} = 0, \tag{2.3}
\]

where \( \beta(a) \) is the QCD \( \beta \)-function, defined as:

\[
-\mu \frac{da}{d\mu} = \beta(a) = \beta_1 a^2 + \beta_2 a^3 + \beta_3 a^4 + \beta_4 a^5 + \ldots. \tag{2.4}
\]

Numerically, for \( N_c = 3 \) and in the \( \overline{\text{MS}} \)-scheme [27] the first four coefficients are given by [28–30]:

\[
\beta_1 = \frac{11}{2} - \frac{1}{3} N_f, \quad \beta_2 = \frac{51}{4} - \frac{19}{12} N_f, \quad \beta_3 = \frac{2857}{64} - \frac{5033}{576} N_f + \frac{325}{1728} N_f^2, \quad \beta_4 = \frac{149753}{768} + \frac{891}{32} \zeta_3 - \left( \frac{1078361}{207360} + \frac{1627}{864} \zeta_3 \right) N_f + \left( \frac{50065}{207360} + \frac{809}{1296} \zeta_3 \right) N_f^2 + \frac{1093}{93312} N_f^3. \tag{2.5}
\]

\(^4\)Since in the rest of this work, we will only be concerned with the vector correlator, the superscript \( V \) will be dropped, and also the flavour content does not matter in the limit of vanishing quark masses.
The RGE puts constraints on the coefficients \( c_{nk} \). Considering the coefficients \( c_{n1} \) to be independent, all other coefficients \( c_{nk} \) with \( k = 2, \ldots, n + 1 \) can be expressed in terms of the \( c_{n1} \) and \( \beta \)-function coefficients. Up to order \( \alpha_s^4 \), the RG constraints lead to:

\[
c_{22} = -\frac{\beta_1}{4} c_{11}, \quad c_{33} = \frac{\beta_1^2}{12} c_{11}, \quad c_{32} = -\frac{1}{4} (\beta_2 c_{11} + 2\beta_1 c_{21}),
\]

\[
c_{44} = -\frac{\beta_3}{32} c_{11}, \quad c_{43} = \frac{\beta_3}{24} (5\beta_2 c_{11} + 6\beta_1 c_{21}), \quad c_{42} = -\frac{1}{4} (\beta_3 c_{11} + 2\beta_2 c_{21} + 3\beta_1 c_{31}).
\]

Furthermore, the coefficients \( c_{n,n+1} = 0 \) for \( n \geq 1 \). The independent coefficients \( c_{n1} \) are known analytically up to order \( \alpha_s^3 \) \([31, 32]\) and at \( N_c = 3 \) in the \( \overline{\text{MS}} \)-scheme take the following values:

\[
c_{01} = c_{11} = 1, \quad c_{21} = \frac{365}{24} - 11\zeta_3 - \left(\frac{11}{12} - \frac{2}{3}\zeta_3\right) N_f,
\]

\[
c_{31} = \frac{87029}{288} - \frac{1103}{4} \zeta_5 + \frac{275}{6} \zeta_5 - \left(\frac{7847}{216} - \frac{262}{9} \zeta_3 + \frac{25}{9} \zeta_5\right) N_f + \left(\frac{151}{162} - \frac{19}{27} \zeta_3\right) N_f^2.
\]

For the next five- and six-loop coefficients \( c_{41} \) and \( c_{51} \), estimates employing principles of “minimal sensitivity” (PMS) or “fastest apparent convergence” (FAC) \([33, 34]\), together with recently computed terms of order \( \alpha_s^4 N_f^2 \), exist which read \([35, 36]\):

\[
c_{41} = 27 \pm 16, \quad c_{51} = 145 \pm 100.
\]

For illustrative purposes, also the central values of these estimates will be taken into account in the analysis below.

Since the Adler function \( D(s) \) satisfies a homogeneous RGE, the logarithms in eq. (2.2) can be resummed with the choice \( \mu^2 = -s \equiv Q^2 \), leading to the simple expression:

\[
D(Q^2) = \frac{N_c}{12\pi^2} \sum_{n=0}^{\infty} c_{n1} a_Q^n,
\]

where \( a_Q \equiv \alpha_s(Q^2)/\pi \). As is again apparent from this equation, the only physically relevant coefficients are the \( c_{n1} \).

3. Hadronic \( \tau \) decay rate

In principle, now one could proceed by inserting the general expression (2.7) for \( \Pi(s) \) into the contour integral of eq. (1.1). However, it is advantageous to rewrite the FESR for the \( \tau \) decay rate in terms of the Adler function \( D(s) \) by partial integration:

\[
R_\tau^D(s_0) = -6\pi i \oint_{|x|=1} \frac{dx}{x} (1-x)^3 (1+x) D(s_0 x),
\]

with the new dimensionless integration variable being \( x \equiv s/s_0 \). For FOPT, order by order \( R_\tau^{\Pi}(s_0) \) and \( R_\tau^D(s_0) \) can be shown to be identical as they should, but applying CIPT, the

\[\text{In writing eq. (3.1), } |V_{ud}|^2 + |V_{us}|^2 = 1 \text{ has been assumed, which numerically is satisfied rather well.}\]
perturbative expansion for $R_T^I(s_0)$ is less well behaved than the one for $R_T^D(s_0)$. Therefore, only the comparison of $R_T^D(s_0)$ in FOPT and CIPT will be investigated in this work.

Inserting the expression (2.2) for $D(s)$ into the contour integral of eq. (3.1), one finds:

$$R_T^D(s_0) = \frac{N_c}{2\pi i} \sum_{n=0}^{\infty} a_n^2 \sum_{k=1}^{n+1} k c_{nk} \oint_{|x|=1} \frac{dx}{x} (1-x)^3 (1+x) \ln^{k-1} \left( \frac{-s_0 x}{\mu^2} \right)$$

$$= \frac{N_c}{2\pi i} \sum_{n=0}^{\infty} a_n^2 \sum_{k=1}^{n+1} k c_{nk} \sum_{l=0}^{k-1} \left( \frac{k-1}{l} \right) \ln^{k-l-1} \frac{s_0}{\mu^2} \oint_{|x|=1} \frac{dx}{x} (1-x)^3 (1+x) \ln^l (-x)$$

$$= \frac{N_c}{2\pi i} \sum_{n=0}^{\infty} a_n^2 \sum_{k=1}^{n+1} k c_{nk} \sum_{l=0}^{k-1} \left( \frac{k-1}{l} \right) J_l \ln^{k-l-1} \frac{s_0}{\mu^2}.$$  (3.2)

In the last line, the contour integrals $J_l$ are defined by

$$J_l \equiv \frac{1}{2\pi i} \oint_{|x|=1} \frac{dx}{x} (1-x)^3 (1+x) \ln^l (-x) = \frac{1}{2\pi} \left[ I_{l,0} + 2 I_{l,1} - 2 I_{l,3} - I_{l,4} \right],$$  (3.3)

with the required integrals $I_{l,m}$ being given by

$$I_{l,m} = i \int_{-\pi}^{+\pi} \alpha^l e^{im\alpha} d\alpha = i \left( \frac{-1}{m} \right)^{l+1} \Gamma(l+1,-i\alpha m) \bigg|_{-\pi}^{+\pi}$$

$$= (-1)^{l+m} \frac{2l!}{m^{l+2}} \sum_{k=1}^{[(l+1)/2]} (-1)^k \frac{m^{2k-2k-1}}{(2k-1)!}.$$  (3.4)

where $\Gamma(l+1,z)$ is the incomplete Gamma function, $\lfloor n \rfloor$ denotes the integer part of $n$ and $m \geq 1$.

For the case $m = 0$, one obtains $I_{l,0} = \delta^l (1 + (-1)^l) \pi^{l+1}/(l+1)$. Explicitly, the first few of the integrals $J_l$, which are needed up to order $\alpha_s^4$, read:

$$J_0 = 1, \quad J_1 = -\frac{19}{12}, \quad J_2 = \frac{265}{72} - \frac{1}{3} \pi^2, \quad J_3 = -\frac{3355}{288} + \frac{19}{12} \pi^2,$$  (3.5)

in agreement with ref. [26].

As discussed above, the Adler function $D(s)$ is a physical quantity, and thus satisfies a homogeneous RGE. Therefore, the logarithms in eq. (3.2) can be resummed. Let us first concentrate on FO perturbation theory, which amounts to taking the choice $\mu^2 = s_0$ in the last line of (3.2), which then leads to

$$R_T^{D,FO}(s_0) = N_c \sum_{n=0}^{\infty} a_n^2 \sum_{k=1}^{n+1} k c_{nk} J_{k-1},$$  (3.6)

with $a_{s_0} \equiv a(s_0)$. Inserting the relations (2.1) for the $c_{nk}$ together with the corresponding contour integrals $J_{k-1}$, up to order $a_s^4$, this leads to:

$$R_T^{D,FO}(s_0) = N_c \left\{ c_{01} + c_{11} a_{s_0} + \left( c_{21} + \frac{19}{24} \beta_1 c_{11} \right) a_{s_0}^2 \right\}.$$
\[ + \left( c_{31} + \frac{19}{12} \beta_1 c_{21} + \left( \frac{19}{24} \beta_2 + \left( \frac{265}{288} - \frac{\pi^2}{12} \right) \beta_1^2 \right) c_{11} \right) a_{s_0}^3 + \left( c_{41} + \frac{19}{8} \beta_1 c_{31} + \left( \frac{19}{12} \beta_2 + \left( \frac{265}{96} - \frac{\pi^2}{4} \right) \beta_1^2 \right) c_{21} \right) \]

\[ + \left( \frac{19}{24} \beta_3 + \left( \frac{1325}{576} - \frac{5\pi^2}{24} \right) \beta_2 \beta_1 + \left( \frac{3355}{3072} - \frac{19\pi^2}{96} \right) \beta_1^3 \right) c_{11} \right\} a_{s_0}^4 \]  

\[ = N_c \left\{ 1 + a_{s_0} + \left( \frac{769}{48} - 9 \zeta_3 \right) a_{s_0}^2 + \left( \frac{363247}{1152} - \frac{27}{16} \pi^2 - \frac{2071}{8} \zeta_3 + \frac{75}{2} \zeta_5 \right) a_{s_0}^3 \right. \]

\[ + \left( \frac{19907171}{6144} + c_{41} - \frac{22683}{256} \pi^2 - \left( \frac{345405}{128} - \frac{729}{16} \pi^2 \right) \zeta_3 + \frac{12825}{32} \zeta_5 \right) \]  

\[ \left. a_{s_0}^4 \right\} . \] (3.7)

For the second step, the coefficients of the \( \beta \)-function (2.5) as well as the \( c_{n1} \)-coefficients of eq. (2.7) have been employed. An important remark is in order here. As should be clear from eq. (3.7), each order \( n \) in FOPT depends on all coefficients \( c_{1i} \) with \( i \leq n \). This will play a crucial role in what follows. Before analysing the expressions numerically, the second approach of resumming the logarithms, namely CI perturbation theory, will be introduced.

For CIPT, the logarithms in eq. (3.2) should be resummed before performing the contour integral. This can be achieved with the choice \( \mu^2 = -s_0x \) in the first line of (3.2), which yields

\[ R_{\tau}^{D,CI} (s_0) = N_c \sum_{n=0}^{\infty} c_{n1} J_n^a(s_0) . \] (3.9)

Here, the equation has been rewritten in terms of the contour integrals \( J_n^a(s_0) \), defined as:

\[ J_n^a(s_0) = \frac{1}{2\pi i} \oint \frac{dx}{x} (1 - x)^3 (1 + x)^n a^n(-s_0x) . \] (3.10)

In contrast to the FO case, for CIPT each order \( n \) just depends on the corresponding coefficient \( c_{n1} \). Thus, all contributions proportional to the coefficient \( c_{n1} \) which in FOPT appear at all perturbative orders equal or greater to \( n \) are resummed into a single term. This is related to the fact that CIPT resums the running of the QCD coupling along the integration contour in the complex \( s \)-plane. To perform the contour integration, we have to analytically continue the strong coupling \( \alpha_s \) to the complex \( s \)-plane, but this is straightforward since the dependence of \( \alpha_s \) on \( s \) is only logarithmic and it has the same cut structure as \( \Pi(s) \).

**4. A simple example**

Before embarking on the general integrals \( J_n^a(s_0) \), as a first step, let us investigate a simplified example which can be treated fully analytically, namely the case where only the first coefficient of the \( \beta \)-function, \( \beta_1 \), is non-zero, and all higher order \( \beta \)-coefficients vanish.
identically. Then the running coupling in eq. (3.10) can be expressed as

\[ a^n(-s_0 x) = \frac{a^n_{s_0}}{1 + \frac{\beta_1}{2} a_{s_0} \ln(-x)} \], \quad (4.1)\]

and the integrals \( J^n_a(s_0) \) can be calculated analytically with the result:

\[ J^n_a(s_0) = a^n_{s_0} \left[ J_{n,0}(\kappa) + 2J_{n,1}(\kappa) - 2J_{n,3}(\kappa) - J_{n,4}(\kappa) \right] . \quad (4.2)\]

Here, the constant \( \kappa \equiv \beta_1 a_{s_0}/2 \), and the integrals \( J_{n,m}(\kappa) \) are found to be

\[ J_{n,m}(\kappa) = e^{-\frac{m}{\kappa}} (\frac{m}{\kappa})^{n-1} \left[ \text{Ei}(\frac{m}{\kappa}z) - e^{\frac{m}{\kappa}z} \sum_{l=1}^{n-1} \Gamma(l)(\frac{m}{\kappa}z)^l \right]_{z=1+i\pi \kappa}^{z=1-i\pi \kappa} , \quad (4.3)\]

with \( \text{Ei}(z) = \int e^{z}/z \, dz \) being the exponential-integral function and \( m \geq 1 \). Again, the case \( m = 0 \) which is also required has to be treated separately and yields:

\[ J_{1,0}(\kappa) = \frac{1}{2\pi i \kappa} \ln \left( \frac{1 + i\pi \kappa}{1 - i\pi \kappa} \right), \quad n = 1 , \quad (4.4)\]

\[ J_{n,0}(\kappa) = \frac{1}{2\pi i \kappa(n-1)} \left[ (1 - i\pi \kappa)^{1-n} - (1 + i\pi \kappa)^{1-n} \right], \quad n \geq 2 . \quad (4.5)\]

The analytic expressions for the integrals \( J^n_a(s_0) \) can readily be compared with their perturbative expansion which is obtained by expanding eq. (4.1) in powers of \( \kappa = \beta_1 a_{s_0}/2 \), before performing the contour integration:

\[ J^n_a(s_0) = \frac{a^n_{s_0}}{\Gamma(n)} \sum_{l=0}^{\infty} \frac{\Gamma(n + l)}{l!} J_l(-\kappa)^l . \quad (4.6)\]

Employing the asymptotic expansion for the exponential-integral function in eq. (4.3) as well as expanding eqs. (4.3) to (4.5) in powers of \( \kappa \), one can verify the agreement between both representations for \( J^n_a(s_0) \).

Let us now turn to a numerical comparison of CI versus FO perturbation theory in the simplified example. To do this, an input value for \( \alpha_s \) is required and the very recent result \( \alpha_s(M^2_{\tau}) = 0.34 \) [6] will be employed for \( a_{s_0} \). The CI expression of eq. (4.2) and the perturbative expansion of the FO result of eq. (4.6), together with eq. (3.9), then lead to:

\[ R_{\tau, \beta_1}^{\text{D,CI}} = 3 \left[ 1 + 0.1455 + 0.0305 + 0.0136 + 0.0060 + 0.0031 \right] = 3.5961 , \quad (4.7)\]

\[ R_{\tau, \beta_1}^{\text{D,FO}} = 3 \left[ 1 + 0.1082 + 0.0609 + 0.0254 + 0.0082 + 0.0024 \right] = 3.6154 . \quad (4.8)\]

From (4.7) and (4.8) one observes that the CI expansion appears to display a better convergence, although the last included term of the FO expansion is somewhat smaller. Altogether, the difference between the two results amounts to \( 3 \cdot 0.0064 \), about 2-3 times the
last term in both expansions. Thus, the agreement between both approaches to performing
the renormalisation group improvement is reasonably good.

Nevertheless, if we were to assume that all coefficients $c_n$ with $n \geq 6$ vanish identically,
the CI result of eq. (4.7) would represent the complete answer. Then the question arises,
how the FO result approaches this value at higher orders in perturbation theory. Since
with eq. (4.6) an all order expression is at our disposal, the question can be answered by
inserting (4.6) into eq. (3.9) and reexpanding in powers of $a_{s_0}$. The numerical result of this
exercise is displayed in table 1 up to the 32nd order. The entries are the perturbative order
$n$ at the one hand and the corresponding term in the expansion of $R_{\tau, \beta_1}^{D, FO}/3$ on the other.
Therefore, the first five entries agree with the corresponding terms in the square bracket
of eq. (4.8).

By inspecting table 1, it is observed that after the first five positive terms, there are
four terms with negative sign. After that, the sign changes at about every second term.

Table 1: Perturbative order $n$ and corresponding terms in the expansion of $R_{\tau, \beta_1}^{D, FO}/3$.

| Perturbative order $n$ | Corresponding term |
|-----------------------|--------------------|
| 1 | 0.108225 |
| 2 | 0.060933 |
| 3 | 0.025394 |
| 4 | 0.008165 |
| 5 | 0.002419 |
| 6 | -0.000607 |
| 7 | -0.004193 |
| 8 | -0.004669 |
| 9 | -0.000104 |
| 10 | 0.003728 |
| 11 | 0.001815 |
| 12 | -0.001991 |
| 13 | -0.001863 |
| 14 | 0.000850 |
| 15 | 0.001407 |
| 16 | -0.000275 |
| 17 | -0.000939 |
| 18 | 0.000032 |
| 19 | 0.005855 |
| 20 | 0.000051 |
| 21 | -0.000354 |
| 22 | -0.000066 |
| 23 | 0.000209 |
| 24 | 0.000057 |
| 25 | -0.000122 |
| 26 | -0.000043 |
| 27 | 0.000070 |
| 28 | 0.000030 |
| 29 | -0.000040 |
| 30 | -0.000020 |
| 31 | 0.000023 |
| 32 | 0.000013 |

Figure 1: Difference $(R_{\tau, \beta_1}^{D, FO} - R_{\tau, \beta_1}^{D, CI})/3$ as a function of the perturbative order $n$ up to which the
terms in the FOPT series are summed in the example with only $\beta_1$ non-vanishing.
Generally, the size of the terms decreases with increasing order, but not from one term to the next. A graphical account of these findings is presented in figure 1, which shows the difference \((R_{D,\text{FO}}^{\tau,\beta_1} - R_{D,\text{CI}}^{\tau,\beta_1})/3\) as a function of the perturbative order \(n\) up to which the terms in the FOPT series are summed. As can be seen from this figure, the sign changes lead to FO results which oscillate around the CI value. Due to the sign change at about every second term, the oscillation frequency is approximately four perturbative orders. Furthermore, the magnitude of the oscillation is tending towards zero, such that the FO value approaches the CI result at large orders. Incidentally, the maximum of the difference between both approaches is found to appear at the fifth order. Calculating the series up to the 200th order, the series still happens to be convergent, and no sign of a divergent behaviour is observed. As has already been discussed in [26], for \(\kappa < 1/\pi\), which corresponds to \(\alpha_s(M^2) < 2/\beta_1 = 0.44\), the expansion (4.1) converges on the whole unit circle. Thus, also the FO series for \(R_{D,\text{FO}}^{\tau,\beta_1}\) should be convergent for the physical value of \(\alpha_s(M^2)\), at least if only a finite number of \(c_{n1}\) coefficients are included.

5. The general case

In order to tackle the general problem with all \(\beta\)-function coefficients \(\beta_1\) to \(\beta_4\) being unequal to zero, the general expansion of \(a(-s_0x)\) in terms of \(a_{s_0}\) is employed, which takes the form:

\[
a(-s_0x) = a_{s_0} \left[ 1 + \sum_{i=1}^{\infty} \sum_{j=1}^{i} d_{ij} a_{s_0}^i \ln^j(-x) \right]. \tag{5.1}
\]

The coefficients \(d_{ij}\) can be calculated from the RGE for the QCD coupling eq. (2.4). The coefficients of the highest and the lowest power of the logarithm can easily be given for arbitrary order and read \(d_{nn} = (-\beta_1/2)^n\) and \(d_{n1} = -\beta_n/2\). The remaining three coefficients up to fourth order are found to be:

\[
\begin{align*}
    d_{32} &= \frac{5}{8} \beta_1 \beta_2, \\
    d_{43} &= -\frac{13}{24} \beta_1^2 \beta_2, \\
    d_{42} &= \frac{3}{8} (\beta_2^2 + 2 \beta_1 \beta_3).
\end{align*}
\tag{5.2}
\]

In principle – given the necessary computing resources – the coefficients \(d_{ij}\) can be calculated to an arbitrary order, taking into account the known \(\beta\)-function coefficients, and setting the even higher-order ones to zero.

The numerical analysis of the case including all available \(\beta\)-function coefficients proceeds along similar lines as the simplified example in the previous section. For CIPT, now the integrals of eq. (3.10) have to be calculated numerically by plugging a numerical solution of the RGE (2.4) for the running coupling and then performing the contour integration. The FO result can be taken from eq. (3.7). In addition including the fifth-order term, one obtains:

\[
R_{D,\text{CI}}^{\tau} = 3 \left[ 1 + 0.1479 + 0.0297 + 0.0122 + 0.0047 + 0.0019 \right] = 3.5893, \tag{5.3}
\]

\[
R_{D,\text{FO}}^{\tau} = 3 \left[ 1 + 0.1082 + 0.0609 + 0.0334 + 0.0144 + 0.0021 \right] = 3.6571. \tag{5.4}
\]
Table 2: Perturbative order $n$ and corresponding terms in the expansion of $R^{D,FO}_\tau/3$.

|   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|
|   | 0.108225 | 0.060933 | 0.033422 | 0.014405 | 0.002052 | -0.006847 | -0.012518 | -0.012029 |
| 9 | -0.004380 | 0.005429 | 0.010012 | 0.006522 | -0.001223 | -0.006793 | -0.006409 | -0.001148 |
| 17| 0.004472 | 0.005997 | 0.002420 | -0.003022 | -0.005577 | -0.003107 | 0.002045 | 0.005211 |
| 25| 0.003582 | -0.001304 | -0.004970 | -0.004026 | 0.000713 | 0.004875 | 0.004498 | -0.000213 |

Again, the CI series displays a better convergence although the last included term in both expansions is almost of the same size. This time, however, the difference between CI and FO perturbation theory looks much more dramatic, as it amounts to $3 \cdot 0.0226$, more than ten times the last included term! This apparent ambiguity in the perturbative prediction of the hadronic $\tau$ decay rate at the moment represents the dominant theoretical uncertainty in the extraction of the strong coupling $\alpha_s$ from this channel.

To gain further insight into the origin of the problem, like in the previous, simplified example, higher order contributions should be inspected. These can be acquired by exploiting the expansion (5.1) for the running coupling in the contour integrals of eq. (3.10) which can be expressed in terms of the $J_l$, and then reexpanding the result in terms of $a_{so}$.$^3$ The result of this exercise is presented in table 4. Like in the last section, after the first five positive terms, there are four negative ones after which the terms change sign at

$^3$Of course, this is just another way of calculating higher order relations for the $c_{n,k}$ coefficients, similar to the ones given in eq. (2.6).

Figure 2: Difference $(R^{D,FO}_\tau - R^{D,CI}_\tau)/3$ as a function of the perturbative order $n$ up to which the terms in the FOPT series are summed.
every third order, and, all in all, decrease in magnitude. The negative sign of the sixth order term, which to some extent already lowers the difference between CIPT and FOPT, has also been observed recently in ref. [5].

Restricting oneself to the five \(c_{n1}\) coefficients discussed above as well as the four known \(\beta\)-function coefficients, again the CI value \((5.3)\) represents the full answer. This time, in figure 2 the difference between the FO expansion summed up to a particular order \(n\) and the complete CI result is displayed up to the 51st order. Until about the 30th order, the series shows the same behaviour as in the simplified example above. It oscillates around the CI result, while approaching it. However, for the general case the convergence to the CI result is much slower, and roughly after the 30th order, an asymptotic behaviour of the series sets in and the terms start to again increase. The observed asymptotic nature of the FOPT series for \(R_{\tau}^{D,FO}\) has nothing to do with the expected asymptotic behaviour of the \(c_{n1}\) coefficients which is due to renormalons \([37, 38]\). Inspection of the expansion \((5.1)\) reveals that for the used physical value of \(\alpha_s(M_{\tau}^2)\), it diverges on part of the unit circle, leading to the behaviour detected in figure 2. The minimal deviation of the FO result at the 30th order is about 0.005, and the oscillation frequency is approximately six perturbative orders. Alas, again the maximum of the deviation occurs at the fifth order.

6. Scale variations

In perturbative QCD calculations, it is quite standard to estimate uncertainties due to as yet uncomputed higher orders by a variation of the in principle arbitrary renormalisation scale. Thus, in this section the influence of scale variations on FO and CI perturbation theory for the hadronic \(\tau\) decay rate shall be investigated. Let us begin with a study of renormalisation group improved FOPT.

Like in ref. [26], the arbitrary renormalisation scale will be introduced by substituting \(\mu^2 = \xi^2 s_0\) in the last line of eq. (3.2), which yields:

\[
R_{\tau}^{D,FO}(\xi^2 s_0) = N_c \sum_{n=0}^{\infty} a^n(\xi^2 s_0) \sum_{k=1}^{n+1} k c_{nk} \sum_{l=0}^{k-1} \binom{k-1}{l} J_l (-2 \ln \xi)^{k-l-1}.
\]

(6.1)

The previous eq. (3.6) just corresponds to the special case \(\xi = 1\). One can then proceed with a numerical analysis, completely analogous to the presentation in the last section. The result of this exercise is shown in figure 3 up to the 60th perturbative order and for two values of \(\xi\). The full triangles correspond to the case \(\xi = 0.9\) whereas the full circles result by setting \(\xi = 1.1\). To guide the eye, the data points have been connected by straight line segments. The required inputs for \(a(\xi^2 M_{\tau}^2)\) have been calculated by solving the RGE (2.4) with the initial value \(\alpha_s(M_{\tau}^2) = 0.34\).

As can be observed from figure 3, changing the renormalisation scale even by only a small amount, the behaviour of the FO series changes quite drastically. In the case of a smaller renormalisation scale \(\xi = 0.9\), the asymptotic behaviour already sets in around the 15th order, and the minimal deviation from the CI result is as large as 0.014, while for the case of a larger renormalisation scale \(\xi = 1.1\), close inspection shows that the amplitude of
the oscillations decreases until about the 45th order after which it gradually again increases. This time the minimal amplitude turns out to be 0.0013. Like in the case $\xi = 1$, however, for both examples the oscillation frequency is about six perturbative orders. Therefore, again for values of the renormalisation scale different from $\xi = 1$, the FOPT series is found to be compatible with the CIPT value (5.3), although due to its rather bad behaviour it should not be utilised for any phenomenological analysis.

For CIPT, introducing an arbitrary renormalisation scale parameter $\xi$ can be achieved with the choice $\mu^2 = -\xi^2 s_0 x$ in the first line of (3.2), which results in

$$R_{\tau}^{D,CI}(\xi^2 s_0) = N_c \sum_{n=0}^{\infty} J_n^a(\xi^2 s_0) \sum_{k=1}^{n+1} k c_{nk}(-2 \ln \xi)^{k-1}. \quad (6.2)$$

This time, the equation has been rewritten in terms of the contour integrals $J_n^a(\xi^2 s_0)$, given by:

$$J_n^a(\xi^2 s_0) \equiv \frac{1}{2\pi i} \oint_{|x|=1} \frac{dx}{x} (1 - x)^3 (1 + x) a^n(-\xi^2 s_0 x). \quad (6.3)$$

From eq. (6.2) it is apparent that in contrast to CIPT with $\xi = 1$ of eq. (3.9), and similarly to FOPT, at a given order $n$, via the coefficients $c_{nk}$, all independent coefficients $c_{i1}$ with $i \leq n$ contribute. Even if again only the first five $c_{i1}$ are assumed to be non-zero, nevertheless, the CIPT series for general $\xi$ does not terminate at this order. Hence, now also for CIPT one can investigate the difference between $R_{\tau}^{D,CI}(\xi^2 s_0)$ for a given $\xi$ and the complete result $R_{\tau}^{D,CI}$ of eq. (5.3).

The result of this exercise is displayed in figure 4 up to the 20th perturbative order. The full triangles now correspond to the case $\xi = 0.5$ whereas the full circles result by
setting $\xi = 2.0$. To guide the eye, the data points have been connected by straight line segments. Generally, the CIPT for arbitrary $\xi$ is much more stable against a variation of the scale parameter than the corresponding FO series. Thus, a larger variation of $\xi$ could be considered. In the case of the smaller $\xi = 0.5$, surprisingly, and most probably by chance, between the second and the fifth order, eq. (6.2) already gives a rather good approximation to the full answer. Beginning with the sixth order, the deviation again fluctuates more strongly until it finally converges towards the result of eq. (5.3) for even higher orders. In the case of a larger scale with $\xi = 2.0$, the approach towards the complete result is much more smooth. Coming from below, the difference only assumes small positive values before again approaching zero. Nevertheless, like for utilising FOPT, there is no real incentive to employ CIPT with values for $\xi$ different from one. This procedure only reshuffles the perturbative expansion, thereby transferring known contributions to higher orders which can as well be resummed.

After the discussion of renormalisation scale dependence of FOPT and CIPT, let us now address the important question which are the uncertainties of the result (5.3) and how they might be estimated. Obviously, one source of uncertainty resides in the contribution of yet uncalculated higher order coefficients $c_{n1}$. Schemes to estimate these coefficients have been discussed in the literature [33–36] (and references therein), but it seems fair to say that no rigorous assessment of the corresponding uncertainty exists, prior to an explicit calculation of a certain coefficient. It also remains unclear if using the size of the last computed term as an estimation for yet higher order contributions is justified – although this is often done in practice. On the other hand, a variation of the renormalisation scale only amounts to a reordering of the perturbative expansion for a given set of known $c_{n1}$ coefficients and

---

4Such estimates for the coefficients $c_{41}$ and $c_{51}$ had been employed above.
has nothing to do with the uncertainty due to so far uncalculated coefficients. This is somewhat different for a change of the renormalisation scheme, as will be discussed in the next section.

A second source of uncertainty in CIPT results from the fact that the running of the QCD coupling is required while integrating over the contour in the complex s-plane, and the perturbative expansion for the β-function has been truncated at the fourth order. An indication of the corresponding uncertainty can be gained by comparing the result (5.3) with the value that would be obtained while using three-loop running for α_s. Numerically, the difference between both approaches is found to be $3 \cdot 0.00099$, only about half of the last included term in the perturbative series. The third, and final uncertainty on the result (5.3) comes from the error of the input value for α_s($M^2$). This uncertainty, however, can be worked out straightforwardly, assuming a given error on α_s($M^2$).

### 7. Scheme variations

Besides investigating the dependence of the perturbative expansion on the choice of the renormalisation scale, also a modification of the renormalisation scheme provides interesting further information. In analogy to the general expression (5.1) for the shift of the scale at which the QCD coupling is evaluated, a transformation of the renormalisation scheme can be represented by the following equation:

$$\tilde{a}_{s_0} = a_{s_0} \left[ 1 + \sum_{i=1}^{\infty} d_i a_{s_0}^i \right].$$

(7.1)

As before, initial quantities, like the coupling $a_{s_0}$, are given in the $\overline{\text{MS}}$-scheme, whereas tilded quantities will always correspond to the transformed scheme. For the case of the modification of the renormalisation scheme, the same scale $s_0$ is assumed in both couplings $a_{s_0}$ and $\tilde{a}_{s_0}$. In principle, one could have considered both transformations simultaneously, in which case the coefficients $d_i$ would have corresponded to coefficients $d_{i0}$ in eq. (5.1), but it appears more transparent to discuss them separately.

Because the Adler function is a physical quantity, it should not depend on the renormalisation scheme used. This can only be true, if together with the coupling also the coefficients of the perturbative expansion $c_{n1}$ get modified. Comparing in eq. (2.2) or (3.10) the expansion in terms of the two schemes, it is straightforward to read off the transformed coefficients [34]. The scheme dependence of the coefficients only starts at order $a^2$, which implies $\tilde{c}_{01} = c_{01}$ and $\tilde{c}_{11} = c_{11}$. Up to order $a^5$ the remaining relations are found to be:

$$\tilde{c}_{21} = c_{21} - d_1 c_{11}, \quad \tilde{c}_{31} = c_{31} - 2d_1 c_{21} + (2d_1^2 - d_2) c_{11},$$

$$\tilde{c}_{41} = c_{41} - 3d_1 c_{31} + (5d_1^2 - 2d_2) c_{21} - (5d_1^3 - 5d_1 d_2 + d_3) c_{11},$$

$$\tilde{c}_{51} = c_{51} - 4d_1 c_{41} + (9d_1^2 - 3d_2) c_{31} - (14d_1^3 - 12d_1 d_2 + 2d_3) c_{21} + (14d_1^4 - 21d_1^2 d_2 + 3d_2^2 + 6d_1 d_3 - d_4) c_{11}.$$
This shows that, even though CIPT still takes the functional form of eq. (3.9), now expressed in terms of the new coefficients $\tilde{\beta}_{n1}$ as well as new contour integrals $\tilde{J}_n^{\alpha}(s_0)$, assuming the series to terminate in one scheme, this is no longer the case in a different scheme. Through relations of the type (7.2), coefficients $\tilde{c}_{n1}$ are generated to all orders. However, to be able to tell in which scheme a certain coefficient $c_{n1}$ vanishes, it necessarily has to be calculated in at least one reference scheme.

Like for eq. (7.2), it is a simple matter to derive from (7.1) the RGE for the coupling $\tilde{\alpha}_{s_0}$ and the corresponding $\beta$-function coefficients $\tilde{\beta}_i$. Thereby, one can confirm the well-known fact that the first two coefficients of the $\beta$-function are independent of the renormalisation scheme, i.e. $\tilde{\beta}_1 = \beta_1$ and $\tilde{\beta}_2 = \beta_2$.\footnote{At least in renormalisation schemes which are mass and gauge-parameter independent [39].} Starting with $\tilde{\beta}_3$, it is found that the $\tilde{\beta}$ coefficients depend on the $d_i$, such that the coefficient $\tilde{\beta}_k$ depends on all $d_i$ with $i = 1, \ldots, k - 1$. Explicitly, the relations for $\tilde{\beta}_3$ and $\tilde{\beta}_4$ take the form:

$$
\tilde{\beta}_3 = \beta_3 - d_1 \beta_2 - (d_1^2 - d_2) \beta_1, \quad \tilde{\beta}_4 = \beta_4 - 2d_1 \beta_3 + d_1^2 \beta_2 + (4d_1^3 - 6d_1d_2 + 2d_3) \beta_1. \quad (7.3)
$$

Again, one could define a scheme, in which all $\tilde{\beta}_k = 0$ for $k \geq 3$ [40]. But in order to do this, one needs to know the $\beta$-function coefficients in one reference scheme.

Let us now proceed with a numerical analysis of the scheme dependence. The principle of minimal sensitivity (PMS) [33] attaches a special importance to the point where the scheme transformation is of a similar size as the expected uncertainty from higher orders in the $\beta$-function, considered in the last section. Furthermore, the “optimal” scheme, where the dependence on the parameters $d_i$ is weakest lies rather close to the $\overline{\text{MS}}$ scheme in which

$$
\beta_i = 0
$$

(1) The scheme transformation stays perturbative, a reasonable choice for the variation of the $d_i$ seems to be the range $-1 \leq d_i \leq 1$, such that the correction is always at most about 10% of the previous term. The variation of $d_1$ is given by the solid line, with the maximum being at $d_1 = 0.165$. Next, the variation of $d_2$ is given by the dashed line, with the maximum at $d_2 = 0.210$, and finally the variation of $d_3$ corresponds to the dotted line.

Several remarks are in order. As expected, for higher corrections, the dependence on the scheme parameters $d_i$ gets weaker and weaker, being strongest for $d_1$ and weakest for $d_3$. Actually, varying $d_3$, the change in $R_\tau^{D,\text{CI}}$ is only by one unit in the fifth digit. While varying $d_1$, the maximal difference to the result of eq. (5.3) is given by $3 \cdot 0.00073$. Thus, the scheme variation is of a similar size as the expected uncertainty from higher orders in the $\beta$-function, considered in the last section. Furthermore, the “optimal” scheme, where the dependence on the parameters $d_i$ is weakest lies rather close to the $\overline{\text{MS}}$ scheme in which
Figure 5: $R^{D,CI}$ as a function of the renormalisation scheme parameters $d_1$, $d_2$ and $d_3$. The solid line corresponds to a variation of $d_1$, the dashed line to $d_2$ and the dotted line to $d_3$. 

all $d_i = 0$. Therefore, also the speed of convergence of the CI perturbative series in the $\overline{\text{MS}}$ scheme can be expected to be close to optimal.

8. Conclusions

Until today, the extraction of $\alpha_s$ from the hadronic $\tau$ decay rate is hampered by an apparent ambiguity between performing the renormalisation group improvement of the perturbative series at a fixed order or in the so-called contour-improved scheme [25,26]. This ambiguity represents the dominant theoretical uncertainty for $\alpha_s$ as extracted from hadronic $\tau$ decays.

Further insight into the origin of the problem can be gained by pursuing the fixed-order expansion to larger orders, still staying consistent with the terms that have been resummed in contour-improved perturbation theory. In a simplified example, where only the first coefficient of the $\beta$-function, $\beta_1$, is kept non-vanishing, this could be done analytically in closed form. For the more general case including the four currently known terms of the $\beta$-function, the expansion of the fixed-order result can be calculated to, in principle, arbitrarily high order. The behaviour of the fixed order series in the simple example as well as in the more general case discussed in sections 4 and 5 have been presented in tables 1 and 2 respectively, and graphically illustrated in figures 1 as well as 2.

It is observed that in the full QCD case the fixed-order result oscillates around the contour-improved value with an oscillation frequency of approximately six perturbative orders, converging to it until the 30th order after which an asymptotic behaviour of the series shows up and the terms again increase. Just including five perturbative terms in the fixed-order case happens to turn out most unfortunate, as for this order the deviation between contour-improved and fixed-order results has a maximum. Analysing the comparison of fixed-order as well as contour-improved perturbation theory for an arbitrary renormalisa-
tion scale parameter $\xi$ unequal to one reveals that also in this case both are compatible. However, invoking $\xi \neq 1$ in CIPT reshuffles known contributions to higher orders thus throwing away available information. Changing the renormalisation scheme is a somewhat different issue, for there the independent coefficients $c_{n1}$ themselves get modified. Still, this does not allow for an unambiguous assessment on the uncertainties resulting from so far neglected higher orders.

All the discussion above demonstrates, that the renormalisation group improvement of perturbative series in finite-energy sum rules, like for the hadronic $\tau$ decay rate in particular, should be performed in the contour-improved scheme. This approach also is most natural in the sense that all terms proportional to a particular perturbative coefficient $c_{n1}$ in the correlation function are resummed to yield the contour-improved contribution at order $n$, whereas in the fixed-order approach terms proportional to the coefficient $c_{n1}$ appear at all orders equal or greater to $n$. A discussion of renormalisation group improvement of quark-mass corrections in finite-energy sum rules along similar lines will be presented in a forthcoming publication.

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