

On the flavour dependence of the $\mathcal{O}(\alpha_s^4)$ correction to the relation between running and pole heavy quark masses

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Abstract. Recently the four-loop perturbative QCD contributions to the relations between pole and running masses of charm, bottom and top quarks were evaluated in the $\overline{\text{MS}}$ -scheme with identical numerical error bars. In this work the flavour dependence of the $\mathcal{O}(\alpha_s^4)$ correction to these asymptotic series is obtained in the semi-analytical form with the help of the least squares method. The numerical structure of the corresponding asymptotic perturbative relations between pole and running c , b and t -quark masses is considered and the theoretical errors of the $\mathcal{O}(\alpha_s^4)$ -contributions are discussed. The explicit dependence for these relations on the renormalization scale μ^2 and the flavour number n_f is presented.

PACS. PACS 12.38.-t Quantum Chromodynamics – PACS 12.38.Bx Perturbative calculations

1 Introduction

It is known that quantum chromodynamics (QCD) is the renormalized gauge theory of quantum fields that describes strong interactions of elementary particles and possesses the property of confinement. As a result, it is impossible to observe quarks in a free state. There are three light u , d and s quarks and three heavy c , b and t quarks in nature. Several theoretical definitions of quark masses in the sectors of light and heavy quarks are used in practice (see e.g. [1]). Among them is the notion of the constituent mass, which is used in applications of various non-relativistic quark models. These constituent masses are not directly related to the renormalized quark masses, which enter the QCD Lagrangian. The renormalized quark masses are usually defined in the $\overline{\text{MS}}$ -scheme. The main modern methods of their determinations, including the versions of the QCD sum rules [2], which were previously used for this purpose e.g. in [3],[4],[5] and [6], are described in the brief review [1].

In this work we will concentrate on the semi-analytical evaluation of the flavour dependence of the $\mathcal{O}(\alpha_s^4)$ perturbative QCD correction to the relation between heavy quark masses defined in the on-shell renormalization scheme and their running analogues, defined in the $\overline{\text{MS}}$ -scheme. Since the masses of the bound states of light quarks are strongly related to various non-perturbative effects [7], it is impossible to introduce for them a notion of pole masses, defined in the region of high enough transferred momentum, where non-perturbative effects are less important ¹.

The precise information about the pole and running heavy quark masses is important in various phenomenological analysis. For example, it allows to compare theoretical QCD prediction for the total cross-section of the e^+e^- annihilation into hadrons process with the experimental data, obtained in the energy regions of J/ψ and Υ -mesons production [8]. This comparison was performed with the help of variant of the QCD sum rules, based on the consideration of the moments of the related spectral function. This approach was proposed in [9].

The high-order QCD relations between running and pole heavy quark masses allow also to decrease theoretical uncertainties of the extracted from experimental data Cabibbo-Kobayashi-Maskawa heavy quark matrix elements, and the V_{cb} element in particular. It enters theoretical predictions for the measured at LHCb $B \rightarrow X_c l \bar{\nu}$ decay width. The precise determination of the b quark mass allows to perform careful multi-loop analysis of semileptonic decay widths of the B-meson, which are proportional to the fifth power of the b quark mass [10]. Another important current problem

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¹ In view of this the values of the constituent heavy quark masses do not differ significantly from the pole masses of heavy quarks.

is the accurate determination of the t quark mass. The number of cosmological and particle physics problems, related to the necessity of decreasing theoretical uncertainties of the evaluation of t quark mass, was discussed quite recently [11]. The precise determination of heavy quark masses, which depends on the knowledge of high order perturbative QCD corrections, is not only the theoretically interesting calculation task, but also is related to the number of phenomenologically important on-going analysis of the experimental data, including the ones, obtained at the LHC experiments.

It is worth reminding that the pole and running heavy quark masses are related by the asymptotic sign-constant perturbative series, the nature of which is manifested in the appearance of the infrared renormalon ambiguities [12], [13]. This leads to the theoretical conclusion that within pure perturbation theory (PT) pole masses may be used when the asymptotic structure of these series is not manifesting itself in the truncated perturbative relation between pole and running heavy quark masses. We will study this important theoretical question for c , b and t quarks at the fourth-order level of PT in QCD.

2 The flavour dependence of the $\mathcal{O}(\alpha_s^4)$ QCD expression for \overline{m}_q/M_q : the known results

In order to determine the ratio between the running and pole masses of heavy quarks it is necessary to know the renormalisation mass constants in the $\overline{\text{MS}}$ and on-shell (OS) schemes, which are introduced using the notion of the unrenormalized bare quark mass $m_{0,q}$ and renormalized finite quantities $\overline{m}_q(\mu^2)$ and M_q as

$$m_{0,q} = Z_m^{\overline{\text{MS}}}(\alpha_s)\overline{m}_q(\mu^2) \quad , \quad m_{0,q} = Z_m^{\text{OS}}(M_q^2, \alpha_s)M_q \quad (1)$$

Next we consider the ratio of the $\overline{\text{MS}}$ scheme running and pole heavy quark masses, namely

$$z_m(\mu^2) = \frac{\overline{m}_q(\mu^2)}{M_q} = \frac{Z_m^{\text{OS}}(M_q^2, \alpha_s(\mu^2))}{Z_m^{\overline{\text{MS}}}(\alpha_s(\mu^2))} \quad (2)$$

Here μ is the renormalization scale in the procedure of dimensional regularization [14] with $\varepsilon = (4-D)/2$. As a result of explicit manifestation of the multiplier $\mu^{2\varepsilon}$, which provides correct dimension between the bare and the renormalized QCD coupling constant $\alpha_s(\mu^2)$ in the $\overline{\text{MS}}$ scheme, and of the $M_q^{-2\varepsilon}$ factor, which appears in the OS scheme, the terms in Z_m^{OS} will contain the characteristic logarithms $L = \ln(\mu^2/M_q^2)$. However, the renormalization scale μ is a free parameter and it can be fixed as $\mu^2 = M_q^2$. Fixing this normalization condition in such way we can see that all RG-governed L -dependent terms disappear and the expression for (2) can be expressed through a standard QCD PT series as

$$\frac{\overline{m}_q(M_q^2)}{M_q} = z_m(M_q^2) = 1 + \sum_{i=1}^{\infty} z_m^{(i)} a_s^i(M_q^2) \quad (3)$$

where $a_s = \alpha_s/\pi$. The coefficients $z_m^{(i)}$ can be represented as polynomials in powers of number of lighter quarks n_l as

$$z_m^{(i)} = \sum_{j=0}^{i-1} z_m^{(i,j)} n_l^j \quad (4)$$

where $n_l = n_f - 1$ is related to the flavour number n_f of the considered heavy quark. The first term $z_m^{(1)}$ was calculated in [15]. The expression for $z_m^{(2)}$ was analytically evaluated in [16] and confirmed later in the process of calculations, performed in [17] and [18] respectively. The coefficient $z_m^{(3)}$ was computed in [10] in the analytical form and in [19] with the help of combination of various semi-analytical methods. The results of these two calculations are in agreement with each other. According to (4) the fourth coefficient $z_m^{(4)}$ can be expressed as

$$z_m^{(4)} = z_m^{(40)} + z_m^{(41)} n_l + z_m^{(42)} n_l^2 + z_m^{(43)} n_l^3 \quad (5)$$

The n_l^3 and n_l^2 coefficients in (5) were computed analytically in [20] and the first two terms are not yet known in this form. We will determine them numerically using the mathematically rigorous ordinary least squares (OLS) method.

In the case of the $\text{SU}_c(3)$ gauge group with the values of the Casimir operators $C_F = 4/3$, $C_A = 3$ and Dynkin index $T_F = 1/2$ the results of the analytical calculations [15],[16],[18],[10],[20] read:

$$z_m^{(10)} = -\frac{4}{3} \quad , \quad z_m^{(20)} = -\frac{3019}{288} + \frac{\zeta_3}{6} - \frac{\pi^2 \ln 2}{9} - \frac{\pi^2}{3} \quad , \quad z_m^{(21)} = \frac{71}{144} + \frac{\pi^2}{18} \quad ,$$

$$\begin{aligned}
z_m^{(30)} &= -\frac{9478333}{93312} - \frac{61\zeta_3}{27} - \frac{644201\pi^2}{38880} + \frac{587\pi^2 \ln 2}{162} + \frac{22\pi^2 \ln^2 2}{81} + \frac{1439\pi^2 \zeta_3}{432} \\
&\quad - \frac{1975\zeta_5}{216} + \frac{695\pi^4}{7776} + \frac{55 \ln^4 2}{162} + \frac{220}{27} \text{Li}_4\left(\frac{1}{2}\right), \\
z_m^{(31)} &= \frac{246643}{23328} + \frac{241\zeta_3}{72} + \frac{967\pi^2}{648} + \frac{11\pi^2 \ln 2}{81} \\
&\quad - \frac{2\pi^2 \ln^2 2}{81} - \frac{61\pi^4}{1944} - \frac{\ln^4 2}{81} - \frac{8}{27} \text{Li}_4\left(\frac{1}{2}\right), \\
z_m^{(32)} &= -\frac{2353}{23328} - \frac{7\zeta_3}{54} - \frac{13\pi^2}{324}, \\
z_m^{(43)} &= \frac{42979}{1119744} + \frac{317\zeta_3}{2592} + \frac{89\pi^2}{3888} + \frac{71\pi^4}{25920}, \\
z_m^{(42)} &= -\frac{32420681}{4478976} - \frac{40531\zeta_3}{5184} - \frac{63059\pi^2}{31104} - \frac{103\pi^2 \ln 2}{972} \\
&\quad + \frac{11\pi^2 \ln^2 2}{243} - \frac{2\pi^2 \ln^3 2}{243} - \frac{5\pi^2 \zeta_3}{48} + \frac{241\zeta_5}{216} - \frac{30853\pi^4}{466560} \\
&\quad - \frac{31\pi^4 \ln 2}{9720} + \frac{11 \ln^4 2}{486} - \frac{\ln^5 2}{405} + \frac{44\text{Li}_4(1/2) + 24\text{Li}_5(1/2)}{81}
\end{aligned}$$

Here $\zeta_n = \sum_{k=1}^{\infty} k^{-n}$ is the Riemann zeta-function, $\text{Li}_n(x) = \sum_{k=1}^{\infty} x^k k^{-n}$ is the polylogarithmic function.

Using these analytical results we get the following numerical expressions for the coefficients $z_m^{(i,j)}$:

$$z_m^{(1)} = -\frac{4}{3}, \quad z_m^{(2)} = -14.3323 + 1.04136n_l, \quad (6)$$

$$z_m^{(3)} = -198.706 + 26.9239n_l - 0.65269n_l^2, \quad (7)$$

$$z_m^{(4)} = z_m^{(40)} + z_m^{(41)}n_l - 43.4824n_l^2 + 0.67814n_l^3 \quad (8)$$

Consider now the results of the recent complicated numerical computer calculations [21] of the fourth coefficient $z_m^{(4)}$ at fixed values of n_l , namely

$$z_m^{(4)} \Big|_{n_l=3} = -1744.8 \pm 21.5, \quad (9)$$

$$z_m^{(4)} \Big|_{n_l=4} = -1267.0 \pm 21.5, \quad (10)$$

$$z_m^{(4)} \Big|_{n_l=5} = -859.96 \pm 21.5 \quad (11)$$

where $\sigma_{n_l}=21.5$ are related to the uncertainties of computations of massive four-loop on-shell propagator master integrals, which enter into the procedure of evaluation of (5) at fixed n_l [21].

Note that the presented inaccuracies in (9)-(11) are equal to each other and do not depend on n_l . In view of this surprising from the first glance feature it is worth to describe how they were fixed in the work of [21]. In the process of these computations it was necessary to evaluate 386 on-shell master integrals. However, only 54 integrals were calculated analytically, while the rest of them were computed numerically by means of the FIESTA program, developed in [22],[23],[24]. This program expresses the results for the integrals in the form of their ϵ -expansion with the numerically evaluated coefficients and definite numerical errors. These errors are interpreted as standard deviations and are combined quadratically in the uncertainties for physical result. The final value of σ_{n_l} are defined in [21] by multiplying these uncertainties by the factor five (!?).

From our point of view the n_l -independence of the inaccuracies $\sigma_{n_l}=21.5$ can be explained by the fact that these errors are almost entirely defined by the error of the constant term $z_m^{(40)}$, which is determined by the set of four-loop diagrams without insertion of the fermion loops into gluon propagators, whereas the uncertainties of n_l -dependent $z_m^{(41)}$ -term are negligible. A possible further study of the reliability of this statement may clarify whether the described above feature of numerical calculations performed by the authors of [21] is really n_l -independent.

3 The determination of the analytically unknown four-loop contributions by the least squares method

Let us use the presented in (9)-(11) numerical results to determine the values of the first two analytically unknown coefficients $z_m^{(40)}$ and $z_m^{(41)}$ in (5) by means of the ordinary least squares (OLS) method. This strict mathematical method is known as a standard approach for solution of the overdetermined systems of linear equations and allows to determine errors of the obtained results.

In our case we have overdetermined system of three linear equations with two unknown coefficients $z_m^{(40)}$ and $z_m^{(41)}$. Combining equation (8) with the numerical results of (9)-(11) we get

$$\begin{aligned} z_m^{(40)} + 3z_m^{(41)} &= -1371.77, \\ z_m^{(40)} + 4z_m^{(41)} &= -614.68, \\ z_m^{(40)} + 5z_m^{(41)} &= 142.32 \end{aligned} \tag{12}$$

Within the OLS method one should define the following residuals $\Delta_{l_k} = z_m^{(40)} + z_m^{(41)}n_{l_k} - y_{l_k}$, where index $1 \leq k \leq 3$ denotes the number of the concrete equation in the system (12) and y_{l_k} are the numbers, given in the r.h.s. of these equations, which are determined as $y_{l_k} = z_{m_k}^{(4)} - z_m^{(42)}n_{l_k}^2 - z_m^{(43)}n_{l_k}^3$, where $z_{m_k}^{(4)}$ is the one from the calculated in [21] three concrete expressions for $z_m^{(4)}$ at fixed number of n_l (see (9)-(11)) and $z_m^{(42)}$ and $z_m^{(43)}$ are the known coefficients, which enter (8).

The second important ingredient of the OLS method is the characteristic function, determined by the sum of squared residuals

$$\Phi(z_m^{(40)}, z_m^{(41)}) = \sum_{k=1}^3 \Delta_{l_k}^2 \tag{13}$$

The solution $(z_m^{(40)}, z_m^{(41)})$ of the presented system exists and is defined uniquely. Indeed, the function $\Phi(z_m^{(40)}, z_m^{(41)})$ always has the minimum, determined from the following equations

$$\frac{\partial \Phi}{\partial z_m^{(40)}} = 0, \quad \frac{\partial \Phi}{\partial z_m^{(41)}} = 0 \tag{14}$$

These conditions allow us to find the numerical values for the coefficients $z_m^{(40)}$ and $z_m^{(41)}$. Within the OLS method it is also possible to define for them the following theoretical uncertainties

$$\Delta z_m^{(40)} = \sqrt{\sum_{k=1}^3 \left(\frac{\partial z_m^{(40)}}{\partial y_{l_k}} \Delta y_{l_k} \right)^2} = \frac{\sqrt{\sum_{k=1}^3 n_{l_k}^2} \Delta y_l}{\sqrt{3 \sum_{k=1}^3 n_{l_k}^2 - \left(\sum_{k=1}^3 n_{l_k} \right)^2}} \tag{15}$$

$$\Delta z_m^{(41)} = \sqrt{\sum_{k=1}^3 \left(\frac{\partial z_m^{(41)}}{\partial y_{l_k}} \Delta y_{l_k} \right)^2} = \frac{\sqrt{3} \Delta y_l}{\sqrt{3 \sum_{k=1}^3 n_{l_k}^2 - \left(\sum_{k=1}^3 n_{l_k} \right)^2}} \tag{16}$$

where for each $k=1, 2, 3$ the values $\Delta y_{l_k} \equiv \Delta y_l = \sigma_{n_l} = 21.5$. It is worth emphasizing that errors of the considered by us OLS method can not be eliminated and in addition to the uncertainties, given in (9)-(11), it is necessary to take them into account.

The determined by (14) numerical values of $z_m^{(40)}$ and $z_m^{(41)}$ coefficients with the fixed by (15) and (16) corresponding theoretical uncertainties read:

$$z_m^{(40)} = -3642.9 \pm 62.0, \quad z_m^{(41)} = 757.05 \pm 15.20 \tag{17}$$

In contrast to the results (9)-(11) of [21], where in accordance with our guess, presented above, all uncertainties σ_{n_l} in the determination of $z_m^{(4)}$ at fixed n_l may be associated with the errors of $z_m^{(40)}$ -term, in our results inaccuracies are found not only in the $z_m^{(40)}$ -term, but in n_l -dependent contribution as well (though it is 4 times smaller).

In the case of applications of the OLS method theoretical error of $z_m^{(40)}$ is almost three times larger than the one, presented in [21], and the OLS uncertainty of $z_m^{(41)}$ -term is comparable with σ_{n_l} .

n_l	The QCD $\mathcal{O}(\alpha_s^4)$ relations of M_q to the running masses $\overline{m}_q(M_q^2)$
3	$M_c \approx \overline{m}_c(M_c^2)(1 + 1.3333a_s(M_c^2) + 12.985a_s^2(M_c^2) + 156.07a_s^3(M_c^2) + (2263.4 \pm 76.9)a_s^4(M_c^2))$
4	$M_b \approx \overline{m}_b(M_b^2)(1 + 1.3333a_s(M_b^2) + 11.944a_s^2(M_b^2) + 130.93a_s^3(M_b^2) + (1698.2 \pm 86.8)a_s^4(M_b^2))$
5	$M_t \approx \overline{m}_t(M_t^2)(1 + 1.3333a_s(M_t^2) + 10.903a_s^2(M_t^2) + 107.11a_s^3(M_t^2) + (1209.4 \pm 98.0)a_s^4(M_t^2))$
n_l	The QCD $\mathcal{O}(\alpha_s^4)$ relations of M_q to the running masses $\overline{m}_q(\overline{m}_q^2)$
3	$M_c \approx \overline{m}_c(\overline{m}_c^2)(1 + 1.3333a_s(\overline{m}_c^2) + 10.318a_s^2(\overline{m}_c^2) + 116.49a_s^3(\overline{m}_c^2) + (1691.1 \pm 76.9)a_s^4(\overline{m}_c^2))$
4	$M_b \approx \overline{m}_b(\overline{m}_b^2)(1 + 1.3333a_s(\overline{m}_b^2) + 9.277a_s^2(\overline{m}_b^2) + 94.41a_s^3(\overline{m}_b^2) + (1224.0 \pm 86.8)a_s^4(\overline{m}_b^2))$
5	$M_t \approx \overline{m}_t(\overline{m}_t^2)(1 + 1.3333a_s(\overline{m}_t^2) + 8.236a_s^2(\overline{m}_t^2) + 73.63a_s^3(\overline{m}_t^2) + (827.3 \pm 98.0)a_s^4(\overline{m}_t^2))$

Table 1. The PT QCD relations between pole and the $\overline{\text{MS}}$ -scheme running c , b and t quark masses for two normalization scales.

Theoretical uncertainties in (17) were computed using only *three* available from (12) points, which form a triangle on the plane in coordinates $(n_l; y_l)$. In view of this the errors in (17) may be overestimated². In our studies we do not consider a correlation of these *three* data points. Indeed, the initial quadratic uncertainties σ_{n_l} does not exceed 10-15 % of the r.h.s. expressions in (12). The resulting numbers are small. Therefore we neglect the consideration of the possible correlation of the errors in our final result (17).

Note, that there is a criterion of the quality of the application of the OLS method. It presumes the evaluation of the coefficient r , which is defined as the geometric mean of regression coefficients. In our case it has the following form

$$r = \sqrt{\rho_{n_l y_l} \rho_{y_l n_l}} = \frac{3 \sum_{k=1}^3 n_{l_k} y_{l_k} - \sum_{k=1}^3 n_{l_k} \sum_{k=1}^3 y_{l_k}}{\sqrt{\left(3 \sum_{k=1}^3 n_{l_k}^2 - \left(\sum_{k=1}^3 n_{l_k}\right)^2\right) \left(3 \sum_{k=1}^3 y_{l_k}^2 - \left(\sum_{k=1}^3 y_{l_k}\right)^2\right)}}$$

In the case when $r=1$ the function $y_l(n_l)$ has a precise linear dependence on n_l . In our case we have $r=0.9999$. This means that even in the case of three equations the OLS method is valid, and gives rather realistic results with the related to theoretical errors, which, however, are becoming more realistic in case when it is used the OLS method for solving more than *three* initial points (see Note added).

4 Results and discussions

Taking into account the presented in (6)-(8) numerical expressions of the available results of analytical calculations and the OLS based expression from (17), we arrive to the following $\mathcal{O}(\alpha_s^4)$ relation between pole and the $\overline{\text{MS}}$ -scheme running heavy quark masses:

$$\begin{aligned} M_q &\approx \overline{m}_q(M_q^2)(1 + 1.3333a_s(M_q^2) \\ &+ (-1.0414n_l + 16.110)a_s^2(M_q^2) \\ &+ (0.6527n_l^2 - 29.701n_l + 239.30)a_s^3(M_q^2) \\ &+ (-0.6781n_l^3 + 46.309n_l^2 \\ &- (864.25 \pm 15.20)n_l + (4457.6 \pm 62.0)a_s^4(M_q^2)) \end{aligned} \quad (18)$$

At present it is commonly accepted to present the values of the running heavy quark masses fixed at the renormalization scale $\mu^2 = \overline{m}_q^2$. At the four-loop level they are related to the heavy quark pole masses by the following perturbative expression

$$M_q = \overline{m}_q(\overline{m}_q^2) \left(1 + \sum_{i=1}^4 l_i a_s^i(\overline{m}_q^2) \right) . \quad (19)$$

The coefficients l_i are determined using the RG-based equations, which were used in [25] at the three-loop level and are presented in the Appendix at the four-loop level. Their numerical expressions have the following form:

$$l_1 = \frac{4}{3}, \quad l_2 = 13.4433 - 1.04136n_l, \quad (20)$$

$$l_3 = 190.595 - 26.6551n_l + 0.65269n_l^2, \quad (21)$$

$$\begin{aligned} l_4 &= -86.54 - z_m^{(40)} + (11.221 - z_m^{(41)})n_l \\ &+ 43.3962n_l^2 - 0.67814n_l^3 \end{aligned} \quad (22)$$

² More detailed clarification of this statement is given in Note added at the end of the paper.

where the obtained in this work OLS values for $z_m^{(40)}$ and $z_m^{(41)}$ are presented in (17). Taking them into account we get the following expression for the l_4 -term:

$$l_4 = (3556.4 \pm 62.0) - (745.83 \pm 15.2)n_l + 43.396n_l^2 - 0.6781n_l^3 \quad (23)$$

Here we emphasize again that the resulting uncertainties are contained not only in the n_l independent contribution, but in proportional to n_l coefficient as well. Our result agrees rather well with the independently obtained in [27] by another method following expression

$$l_4 = (3556.5 \pm 21.5) - 745.85n_l + 43.396n_l^2 - 0.6781n_l^3 \quad (24)$$

Both methods of the determination of the n_l -dependence of l_4 have common features. They are using the same input, namely, the results of the performed in [20] analytical calculations of the n_l^2 and n_l^3 $\mathcal{O}(\alpha_s^4)$ coefficients $z_m^{(42)}$ and $z_m^{(43)}$ in the ratio between the $\overline{\text{MS}}$ -scheme running and pole heavy quark masses. Next, both methods are using the obtained in [21] numerical expressions (9)-(11) of the whole values of the four-loop corrections to considered ratios.

However, these two methods are completely different from theoretical point of view. Firstly, in our work we use rather rigorous OLS mathematical method, while the approach of [27] is based on application of less mathematically motivated special fitting procedure, which is supplemented by the extra *theoretical* information, namely by the derived in [28] and [12] renormalon-based large β_0 -representation of the n_l -dependence for the l_4 coefficient³. In our studies it was not necessary to use this additional theoretical input.

Secondly, we apply the OLS method to obtain the numerical values of $z_m^{(40)}$ and $z_m^{(41)}$ contributions to (5), and after this we get the corresponding numerical expression for l_4 (see (22) and (23)) using the appropriate RG-equations. In the work of [27] the analogous expression for l_4 , which is given in (24), was obtained as the result of application of the fitting procedure to the analytical contributions [20] and numerical results of [21], which are related to the n_l -dependence of l_4 -coefficient directly. In view of these two arguments the coincidence of the central values of the n_l -independent and the proportional to the first power of n_l terms in our result (23) and in the similar result (24) from [27] is the non-trivial fact and gives extra confidence in the validity of both mathematical OLS method and this more physical fitting procedure. In addition the OLS based result (23) has the sign-alternating structure of the contributions which are proportional to the powers of n_l . A posteriori this feature of the OLS based results supports the applied in [27] renormalon-based large- β_0 theoretical considerations.

The numerical $\mathcal{O}(\alpha_s^4)$ approximations of the relations between pole and c -, b - and t -quarks running masses are presented in Table 1. The results of Table 1 demonstrate that the general asymptotic structure of the perturbative QCD series really manifest itself. Indeed, one can see that all relations contain sign-constant and significantly growing coefficients of the corresponding PT series. Moreover, the table demonstrates the importance of the four-loop QCD contributions in all given above relations.

Note, that the OLS mathematical method allows to formalize the procedure of fixing theoretical error bars of the $\mathcal{O}(\alpha_s^4)$ coefficients. In the presented in Table 1 relations the obtained by OLS method uncertainties are based on given above equations (15) and (16). As it was already mentioned previously these errors are using only *three* available from the system (12) initial points and may be overestimated.

In the result of applications of the fitting procedure of [27] the error of n_l -independent term in (24) is fixed by the error of the numerical calculations of [21].

Let us now study the concrete behaviour of the QCD PT $\mathcal{O}(\alpha_s^4)$ relation between pole and the $\overline{\text{MS}}$ -scheme running masses of heavy quarks. In our numerical studies we will use the world average values of the running masses of the c and b -quarks, which are given in the review of particle physics properties volume [30], namely $\overline{m}_c(\overline{m}_c^2)=1.275$ GeV and $\overline{m}_b(\overline{m}_b^2)=4.180$ GeV. The value of the running t quark mass $\overline{m}_t(\overline{m}_t^2)=163.643$ GeV is taken from the work [21]. It does not contradict the results presented in PDG, which can be extracted from measurement of $\sigma(t\bar{t})$ in $p\bar{p}$ collisions.

The expression for α_s is defined through the expansion in inverse powers of $L = \ln(\overline{m}_q^2/\Lambda_{\overline{\text{MS}}}^{(n_f)})^2$ terms with the parameters $\Lambda_{\overline{\text{MS}}}^{(n_f)}$, which depend on the flavour number of quarks ($n_f = n_l + 1$) and the order of approximation of the QCD β -function in the $\overline{\text{MS}}$ -scheme. For the b quark we take the average world value of $\Lambda_{\overline{\text{MS}}}^{(n_f=5)}$ from [31], which is consistent with the world average value $\alpha_s(M_Z^2) = 0.1185$. In order to obtain values $\Lambda_{\overline{\text{MS}}, N^3\text{LO}}^{(n_f=4)}$ and $\Lambda_{\overline{\text{MS}}, N^3\text{LO}}^{(n_f=6)}$ we use the $N^3\text{LO}$ matching transformation conditions from [32]. The corresponding results read:

$$\Lambda_{\overline{\text{MS}}, N^3\text{LO}}^{(n_f=4)} = 297 \text{ MeV}, \quad \alpha_s^{N^3\text{LO}}(\overline{m}_c^2) \approx 0.399 \quad (25)$$

³ It is known from [29] that the application of this approach for other physical quantities gives reasonable prediction of the n_l -dependence for the three-loop perturbative QCD approximations.

$$\Lambda_{\overline{\text{MS}}, \text{N}^3\text{LO}}^{(n_f=5)} = 215 \text{ MeV}, \quad \alpha_s^{\text{N}^3\text{LO}}(\overline{m}_b^2) \approx 0.227, \quad (26)$$

$$\Lambda_{\overline{\text{MS}}, \text{N}^3\text{LO}}^{(n_f=6)} = 91 \text{ MeV}, \quad \alpha_s^{\text{N}^3\text{LO}}(\overline{m}_t^2) \approx 0.109 \quad (27)$$

The obtained results for $\Lambda_{\overline{\text{MS}}}^{(n_f=4)}$ and $\Lambda_{\overline{\text{MS}}}^{(n_f=6)}$ are in agreement with the ones, given in [31]. This gives us confidence that the presented above N³LO expressions for α_s at different scales are consistent with the world average value $\alpha_s(M_Z^2)$.

Using the given in Table 1 QCD $\mathcal{O}(\alpha_s^4)$ relations of M_q to the fixed above values of the running masses $\overline{m}_q(\overline{m}_q^2)$ and the results for α_s from (25)-(27) we get the following numerical expressions for the four-loop perturbative series we are interested in

$$\begin{aligned} \frac{M_c}{1 \text{ GeV}} &\approx 1.275 + 0.216 + 0.213 \\ &+ 0.305 + 0.563 \pm 0.026, \end{aligned} \quad (28)$$

$$\begin{aligned} \frac{M_b}{1 \text{ GeV}} &\approx 4.180 + 0.403 + 0.202 \\ &+ 0.149 + 0.140 \pm 0.010, \end{aligned} \quad (29)$$

$$\begin{aligned} \frac{M_t}{1 \text{ GeV}} &\approx 163.643 + 7.549 + 1.613 \\ &+ 0.499 + 0.194 \pm 0.023 = 173.498 \pm 0.023 \end{aligned} \quad (30)$$

where the theoretical OLS inaccuracies of the b and t quark pole masses are 2.5 and 4.6 times larger than the errors, presented in [21]. Indeed, the OLS errors include the uncertainties of [21], given in (9)-(11), as a part of the determination of the theoretical inaccuracies with the help of the OLS method.

All numerical corrections give a significant contributions to the expressions for the pole heavy quark masses. Moreover, in the case of c quark, the asymptotic nature of PT series is manifesting itself from the third order of PT. Indeed, the numerical values of the fourth and fifth terms are larger than the third term, which corresponds to the next-to-leading $\mathcal{O}(\alpha_s^2)$ term. In view of this it is really impossible to fix the value of the pole c quark mass at the fourth and even third level of perturbative QCD. In the case of the b quark the numerical value of the fourth order term is comparable with the $\mathcal{O}(\alpha_s^3)$ contribution. These features demonstrate that the studied theoretically in [12], [13] IR renormalon long-distance contributions to the PT series for the c and b quark pole masses are manifesting themselves rather early, namely at the third and fourth order of corresponding perturbative series. The expression (28) clarifies the known conclusion why instead of the pole c -quark mass it is commonly accepted to use the running c -quark mass in the number of the concrete phenomenological applications. For the b -quark the concept of the pole mass may be still applicable at the truncated $\mathcal{O}(\alpha_s^3)$ perturbative analysis. However, in view of the manifestation of the asymptotic structure of the PT series of (29) at the four-loop level it is indeed more rigorous to use the running b quark mass in the related high-order perturbative QCD phenomenological studies.

In the case of the t -quark mass the evaluated PT QCD corrections are decreasing. However, the effect of $\mathcal{O}(\alpha_s^4)$ correction is not negligible. Its uncertainty was fixed within the OLS approach. The accuracy of our method turns out to be 23 MeV, which is over 5 times larger than the similar theoretical uncertainty, estimated in [21]. The difference may be important in the detailed considerations of the theoretical studies, discussed in [11]. The clarification of the raised in our work problems, related to the determination of real precision of the four-loop QCD contribution to the relation between pole and running t -quark masses are also important in view of the existence of the electro-weak (EW) and mixed EW-QCD corrections to the pole-running t -quark mass relation [26]. These corrections are comparable with the expressions for the four-loop QCD contributions. The discussed in this work theoretical uncertainties can be removed after direct analytical calculation of the $z_m^{(40)}$ and $z_m^{(41)}$ coefficients in (5). The preparations for these calculations have already started [33] from the creation of the first computer program.

5 Conclusion

In this work we determine the constant term $z_m^{(40)}$ and the coefficient $z_m^{(41)}$ of the flavour dependent $\mathcal{O}(\alpha_s^4)$ contribution to the ratio $\overline{m}_q(M_q^2)/M_q$ by the mathematical least squares method (which is not related to any fitting procedure) and evaluate the inaccuracies of these two coefficients using the obtained in [21] *three* given in (9)-(11) numerical expressions. In this case the fixed by the OLS method whole uncertainties of the four-loop corrections to the relation between pole and running heavy quark masses turn out to be 6.5, 2.5 and 4.6 times larger than the estimated in similar errors for the c , b and t quark masses respectively. Theoretical arguments in favour of the applicability of the OLS method for the mathematically consistent determination of the central numerical values of two contributions to

the n_l -dependent expression for the four-loop correction to the relations between pole and the $\overline{\text{MS}}$ -scheme running heavy quark masses are presented. The asymptotic structure of these perturbative relations It will be interesting to understand the reason of differences of the obtained in this work error-bars for the $\mathcal{O}(\alpha_s^4)$ contribution to the ratio between running and pole heavy quark masses from the ones obtained as the result of the performed in [21] important numerical calculations. The necessity of the direct analytical calculation of $z_m^{(40)}$ and $z_m^{(41)}$ terms is emphasized.

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Appendix

Here we describe in details how to obtain the flavour-dependent $\mathcal{O}(\alpha_s^4)$ relation between pole and $\overline{\text{MS}}$ -scheme running masses of heavy quarks, normalized at the non-fixed normalization scale μ^2 . To solve this problem we use the four-loop approximation of the QCD β -function in the $\overline{\text{MS}}$ -like schemes, which is defined as

$$\beta(a_s) = \mu^2 \frac{\partial a_s(\mu^2)}{\partial \mu^2} = - \sum_{i=0}^3 \beta_i a_s^{i+2} \quad (31)$$

The numerical expressions of the coefficients β_i , which are expanded in powers of $n_l = n_f - 1$, have the following form

$$\begin{aligned} \beta_0 &= 2.5833 - 0.16666n_l, \\ \beta_1 &= 5.5833 - 0.79166n_l, \\ \beta_2 &= 18.045 - 4.1808n_l + 0.09403n_l^2, \\ \beta_3 &= 88.684 - 23.951n_l + 1.5999n_l^2 + 0.00585n_l^3 \end{aligned}$$

The scheme-independent coefficients β_0 and β_1 were analytically evaluated in [34],[35] and [36],[37],[38] respectively. The scheme-dependent coefficients β_2 and β_3 are known from the symbolical calculations, which were done in [39],[40] and [41],[42] correspondingly.

The solution of the RG-equation (31), namely

$$\ln \frac{\mu^2}{M_q^2} = \int_{a_s(\mu^2)}^{a_s(M_q^2)} \frac{dx}{\beta_0 x^2 + \beta_1 x^3 + \beta_2 x^4 + \beta_3 x^5}$$

can be expressed through the ln-dependent terms c_1 - c_4 . They have the following form

$$\begin{aligned} c_1 &= \beta_0 \ln \frac{\mu^2}{M_q^2}, \quad c_2 = \beta_0^2 \ln^2 \frac{\mu^2}{M_q^2} + \beta_1 \ln \frac{\mu^2}{M_q^2}, \\ c_3 &= \beta_0^3 \ln^3 \frac{\mu^2}{M_q^2} + \frac{5}{2} \beta_0 \beta_1 \ln^2 \frac{\mu^2}{M_q^2} + \beta_2 \ln \frac{\mu^2}{M_q^2}, \\ c_4 &= \beta_0^4 \ln^4 \frac{\mu^2}{M_q^2} + \frac{13}{3} \beta_1 \beta_0^2 \ln^3 \frac{\mu^2}{M_q^2} \\ &\quad + \frac{3}{2} (\beta_1^2 + 2\beta_0 \beta_2) \ln^2 \frac{\mu^2}{M_q^2} + \beta_3 \ln \frac{\mu^2}{M_q^2} \end{aligned}$$

We will also use the four-loop approximation of the anomalous mass dimension in the $\overline{\text{MS}}$ -scheme, which is defined as

$$\gamma_m(a_s) = \mu^2 \frac{\partial \ln(\overline{m}_q(\mu^2))}{\partial \mu^2} = - \sum_{i=0}^3 \gamma_i a_s^{i+1} \quad (32)$$

The numerical expressions of its coefficients in powers of n_l have the following form

$$\begin{aligned} \gamma_0 &= 1, \\ \gamma_1 &= 4.0694 - 0.13888n_l, \\ \gamma_2 &= 17.204 - 2.3381n_l - 0.02700n_l^2, \\ \gamma_3 &= 80.117 - 18.537n_l + 0.2935n_l^2 + 0.00579n_l^3. \end{aligned}$$

The first scheme-independent coefficient γ_0 was calculated in the works [36],[37]. The presented above $\overline{\text{MS}}$ -scheme results for γ_1 and γ_2 follow from the analytical calculations, performed in [15],[43] and [44], [45] respectively. The n_l -dependence for the term γ_4 is obtained from its analytical expression, simultaneously evaluated in [46] and [47].

The solution of the RG-equation for the running mass reads

$$\frac{\overline{m}_q(M_q^2)}{\overline{m}_q(\mu^2)} = \exp \left(\int_{a_s(\mu^2)}^{a_s(M_q^2)} \frac{\gamma_m(x) dx}{\beta(x)} \right) \quad (33)$$

It can be expressed through the following terms

$$\begin{aligned} b_1 &= \gamma_0 \ln \frac{\mu^2}{M_q^2}, \\ b_2 &= \frac{1}{2} \gamma_0 (\gamma_0 + \beta_0) \ln^2 \frac{\mu^2}{M_q^2} + \gamma_1 \ln \frac{\mu^2}{M_q^2}, \\ b_3 &= \frac{1}{3} \gamma_0 (\beta_0 + \gamma_0) (\beta_0 + \gamma_0 / 2) \ln^3 \frac{\mu^2}{M_q^2} \\ &\quad + \frac{1}{2} (\beta_1 \gamma_0 + 2\gamma_1 (\beta_0 + \gamma_0)) \ln^2 \frac{\mu^2}{M_q^2} + \gamma_2 \ln \frac{\mu^2}{M_q^2}, \\ b_4 &= \frac{1}{24} (6\gamma_0 \beta_0^3 + 11\gamma_0^2 \beta_0^2 + 6\gamma_0^3 \beta_0 + \gamma_0^4) \ln^4 \frac{\mu^2}{M_q^2} \\ &\quad + \frac{1}{6} (5\gamma_0 \beta_0 \beta_1 + 3\gamma_0^2 \beta_1 + 3\gamma_0^2 \gamma_1 + 6\gamma_1 \beta_0^2) \\ &\quad + 9\gamma_0 \gamma_1 \beta_0 \ln^3 \frac{\mu^2}{M_q^2} + \frac{1}{2} (\gamma_0 \beta_2 + 2\gamma_1 \beta_1 + 3\gamma_2 \beta_0) \\ &\quad + 2\gamma_0 \gamma_2 + \gamma_1^2 \ln^2 \frac{\mu^2}{M_q^2} + \gamma_3 \ln \frac{\mu^2}{M_q^2} \end{aligned}$$

Together with the derived above c_1 - c_4 expressions, they contribute to the \ln -dependent representation for the coefficients $l_1(\mu^2)$ - $l_4(\mu^2)$ in the analogous to (19) relation between pole and $\overline{\text{MS}}$ -scheme running heavy quark masses, normalized at the arbitrary renormalization scale:

$$\begin{aligned} l_1 &= b_1 - z_m^{(1)}, \\ l_2 &= b_2 - z_m^{(1)}(b_1 + c_1) + (z_m^{(1)})^2 - z_m^{(2)}, \\ l_3 &= b_3 + ((z_m^{(1)})^2 - z_m^{(2)})(b_1 + 2c_1) \\ &\quad - z_m^{(1)}(b_2 + c_2 + b_1 c_1) - (z_m^{(1)})^3 + 2z_m^{(1)} z_m^{(2)} - z_m^{(3)}, \\ l_4 &= b_4 - ((z_m^{(1)})^3 - 2z_m^{(1)} z_m^{(2)} + z_m^{(3)})(b_1 + 3c_1) \\ &\quad + ((z_m^{(1)})^2 - z_m^{(2)})(b_2 + 2c_2 + 2b_1 c_1 + c_1^2) \\ &\quad - z_m^{(1)}(b_3 + c_3 + b_2 c_1 + b_1 c_2) \\ &\quad + (z_m^{(1)})^4 - 3(z_m^{(1)})^2 z_m^{(2)} + 2z_m^{(1)} z_m^{(3)} + (z_m^{(2)})^2 - z_m^{(4)}. \end{aligned} \quad (34)$$

The numerical expressions for the coefficients $z_m^{(i)}$ with $1 \leq i \leq 4$ are presented in (6),(7) and (8). The results for the terms $z_m^{(40)}$ and $z_m^{(41)}$ with their related uncertainties were obtained in the main part of the work with the help of mathematically rigorous OLS method and are given in (17). Substituting now the presented above expressions for the coefficients of the QCD RG-functions $\beta(a_s)$ and $\gamma_m(a_s)$ into the defined above \ln -dependent terms c_1 - c_4 and b_1 - b_4 , which enter in the equations (34), we get the following final expression for the the flavour-dependent $\mathcal{O}(\alpha_s^4)$ explicit relation between pole and $\overline{\text{MS}}$ -scheme running masses of heavy quarks at the arbitrary renormalization scale μ^2 :

$$\begin{aligned} M_q &= \overline{m}_q(\mu^2) \left[1 + \left(\frac{4}{3} + \ln \frac{\mu^2}{M_q^2} \right) a_s(\mu^2) \right. \\ &\quad \left. + \left(16.110 - 1.0413n_l + (8.8471 - 0.36109n_l) \ln \frac{\mu^2}{M_q^2} \right) a_s^2(\mu^2) \right] \end{aligned}$$

$$\begin{aligned}
& + (1.79166 - 0.083333n_l) \ln^2 \frac{\mu^2}{M_q^2} \Big) a_s^2(\mu^2) \\
& + \left(239.29 - 29.700n_l + 0.6526n_l^2 \right. \tag{35}
\end{aligned}$$

$$\begin{aligned}
& + (129.408 - 15.3671n_l + 0.31996n_l^2) \ln \frac{\mu^2}{M_q^2} \\
& + (32.1047 - 3.05309n_l + 0.060179n_l^2) \ln^2 \frac{\mu^2}{M_q^2} \\
& + (3.68286 - 0.370369n_l + 0.0092591n_l^2) \ln^3 \frac{\mu^2}{M_q^2} \Big) a_s^3(\mu^2) \\
& + \left(4457.6 \pm 62.0 - (864.25 \pm 15.20)n_l + 46.309n_l^2 \right. \tag{36} \\
& - 0.6781n_l^3 + (2463.69 - 449.525n_l + 22.6677n_l^2 \\
& - 0.31920n_l^3) \ln \frac{\mu^2}{M_q^2} + (651.105 - 113.1880n_l \\
& + 5.58420n_l^2 - 0.079958n_l^3) \ln^2 \frac{\mu^2}{M_q^2} + (102.7368 \\
& - 15.70710n_l + 0.732188n_l^2 - 0.0100295n_l^3) \ln^3 \frac{\mu^2}{M_q^2} \\
& + (8.05625 - 1.270540n_l + 0.0665503n_l^2 \\
& \left. - 0.00115739n_l^3) \ln^4 \frac{\mu^2}{M_q^2} \Big) a_s^4(\mu^2) + \mathcal{O}(a_s^5) \right]
\end{aligned}$$

At fixed $n_l = 3, 4, 5$ the expressions of the terms, contributing to l_4 agree with the results of [21].

Note added

After two previous versions of this work were submitted for publication the detailed description of the numerical calculations of [21] appeared in [48], where the authors clarified the number of questions, raised in this work and in the talk [49]. The new work [48] presented 21 more precise numerical expressions for $z_m^{(4)}$ -coefficient at fixed n_l values, which vary in the region $0 \leq n_l \leq 20$. For these data set the OLS method gives the more precise analogs of the terms, obtained above in (17) from three given in [48] terms only, namely $z_m^{(40)} = -3654.14 \pm 0.76$, $z_m^{(41)} = 756.94 \pm 0.07$. Their central values coincide with the presented in [48] results of the diagram-by-diagram calculations. One can see that as the result of taking extra 18 numerical expressions, given in [48] the uncertainties of the OLS method are decreasing significantly and are becoming more physical. The more precise OLS values of the terms, determined above in (24) and (36) using three equations only, read $l_4 = (3567.6 \pm 0.76) - (745.72 \pm 0.07)n_l + 43.396n_l^2 - 0.6781n_l^3$ and $d_4 = 4469.04 \pm 0.76 - (864.14 \pm 0.07)n_l + 46.307n_l^2 - 0.6781n_l^3$. The presented OLS-based expression for l_4 is in the excellent agreement with the result of numerical diagram-by-diagram calculations, given in [48]. The central values of the two OLS-determined terms also agree rather well with similar values of the same terms from (24) and (36), obtained by us in the main part of this work. The agreement of the results obtained in this work by means of mathematically consistent OLS method with the results of diagram-by-diagram calculations, which were presented only recently in [48], should be considered as the argument in favour of self-consistency of the performed at supercomputer Lomonosov of MSU complicated and important numerical calculations, described in [21], [48], and may be used in various physical and mathematical studies.

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