Top mass determination and $O(\alpha_5^5 m)$ correction to toponium $1S$ energy level

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**Abstract**

Recently the full $O(\alpha_5^5 m, \alpha_5^5 m \log \alpha_S)$ correction to the heavy quarkonium $1S$ energy level has been computed (except the $\alpha_3$-term in the QCD potential). We point out that the full correction (including the $\log \alpha_S$-term) is approximated well by the large-$\beta_0$ approximation. Based on the assumption that this feature holds up to higher orders, we discuss why the top quark pole mass cannot be determined to better than $O(\Lambda_{QCD})$ accuracy at a future $e^+e^-$ collider, while the $\overline{\text{MS}}$ mass can be determined to about 40 MeV accuracy (provided the 4-loop $\overline{\text{MS}}$-pole mass relation will be computed in due time).
Recently a large part of the $\mathcal{O}(\alpha_S^5 m)$ corrections [1,2] to the energy spectrum of the heavy quarkonium 1$S$ state has been calculated. Combining this with the previously known $\mathcal{O}(\alpha_S^5 m \log \alpha_S)$ corrections [3,4] the only remaining piece to be computed in order to complete the $\mathcal{O}(\alpha_S^5 m)$ corrections is the non-logarithmic term ($a_3$) of the static QCD potential at 3-loop. Using a Padé estimate [5] of $a_3$, Ref. [2] examined the scale dependences and the convergence properties of the bottomonium 1$S$ and the (would-be) toponium 1$S$ energy levels. The dependences of the energy levels on the value of $a_3$ are found to be rather weak. As for the toponium case, Ref. [2] concluded that the top quark pole mass can be extracted from the 1$S$ energy level with a theoretical error of about 80 MeV. This estimate of the theoretical error on the top quark pole mass appears to be considerably smaller as compared to a previous common consensus that the pole mass has a theoretical uncertainty of order $\Lambda_{QCD} \sim 200–300$ MeV [6].

In this paper we discuss two issues. First we point out that the presently known $\mathcal{O}(\alpha_S^5 m)$ correction to the 1$S$ energy level is approximated fairly well by its large-$\beta_0$ approximation (naive nonabelianization) [7]. We consider this fact to be quite non-trivial because of the following reason. We know that from $\mathcal{O}(\alpha_S^5 m)$ the ultrasoft scale starts to contribute to the energy level. Since it is a completely new type of contribution (as compared to the lower-order corrections), and since it is generally believed to give very large corrections [3,4], we have expected that the large-$\beta_0$ approximation may well fail to be a good approximation at $\mathcal{O}(\alpha_S^5 m)$ in the energy level.

One may wonder that our point, that the large-$\beta_0$ approximation is good, is in contradiction to the conclusion of [2]: “We have found that the N$^3$LO corrections are dominated neither by logarithmically enhanced $\alpha_S^3 \ln(\alpha_S)$ nor by the renormalon induced $\beta_0^3 \alpha_S^3$ terms and thus the full calculation of the correction is crucial for quantitative analysis.” In fact, there is no contradiction, because the definition of the “$\beta_0^3 \alpha_S^3$ terms” in [2] differs from that of the usual large-$\beta_0$ approximation.* Nevertheless, we have to say that the above statement of [2] is quite misleading, since it does not address the difference between its $\beta_0^3 \alpha_S^3$ terms and the large-$\beta_0$ approximation, and since it is the large-$\beta_0$ approximation that is the empirically successful approximation and, therefore, the renormalon dominance picture has often been discussed in this context in the literature.

Secondly, we discuss an error estimate of the top quark pole mass based on the assumption that the large-$\beta_0$ approximation continues to be a good approximation up to higher orders. At the same time we discuss the accuracy with which the top quark $\overline{\text{MS}}$ mass can be extracted from the toponium 1$S$ energy level.

The sum of the full $\mathcal{O}(\alpha_S^5 m)$ and $\mathcal{O}(\alpha_S^5 m \log \alpha_S)$ corrections to the energy level of the heavy quarkonium 1$S$ state is given in Eqs. (6), (12) and (13) of [2]. The part unrelated to the lower-order corrections via the renormalization-group equation (for the running of the coupling) can be extracted by setting $L_\mu = \log[\mu/(C_F \alpha_S(\mu)m_{\text{pole}})] = 0$. It reads numerically

$$
\delta E_1^{(3)} \bigg|_{L_\mu=0} = -\frac{(C_F \alpha_S(\mu))^2}{4} m_{\text{pole}} \times \left(\frac{\alpha_S(\mu)}{\pi}\right)^3 c_3,
$$

$$
c_3 \approx 7078.8 + 0.03125 a_3 - 1215.5 n_f + 69.451 n_f^2 - 1.2147 n_f^3 + 474.29 \log(\alpha_S(\mu)),
$$

*For instance, the term proportional to $a_1 \beta_0^2$ is not included in the $\beta_0^3$ term of [2], whereas a part of $a_1 \beta_0^3$ is included in the large-$\beta_0$ approximation.
Table 1: Numerical values of $c_3$ and its large-$\beta_0$ results are shown for $\alpha_S = 0.1, 0.2, 0.3$ and $n_f = 4, 5$. For each $c_3$(large-$\beta_0$), the ratio to the full result $(c_3)$ is shown in the parenthesis. The Padé estimate [5] of $a_3$ is used in Eq. (2) to obtain $c_3$.

where $C_F = 4/3$ is a color factor.

In general, the large-$\beta_0$ approximation of a quantity, at a given order of perturbative expansion in $\alpha_S$, is defined as follows: We first compute the leading order contribution in an expansion in $1/n_f$, where $n_f$ is the number of light quark flavors, which comes from so-called bubble chain diagrams. Then we transform this large $n_f$ result by a simplistic replacement $n_f \to n_f - 33/2 = -(3/2)\beta_0$. In many phenomenological applications the large-$\beta_0$ approximation turns out to be a good approximation of the full result for quantities which contain the leading renormalon, see e.g. [8, 9, 10, 11]. The corresponding correction to Eq. (2) in the large-$\beta_0$ approximation is given by [12, 13]

$$c_3(\text{large-$\beta_0$}) = \beta_0^3 \left( \frac{517}{864} + \frac{19\pi^2}{144} + \frac{11 \zeta_3}{6} + \frac{\pi^4}{1440} - \frac{\pi^2 \zeta_3}{8} + \frac{3 \zeta_5}{2} \right)$$

$$\approx 5649.36 - 1027.16 n_f + 62.2519 n_f^2 - 1.25761 n_f^3.$$ (3)

In Table I we compare $c_3$ and $c_3$(large-$\beta_0$) for values of $n_f$ and $\alpha_S$ corresponding to the $\Upsilon(1S)$ and toponium 1S states. For $a_3$, we used the Padé estimate [5] as well as the estimate based on the renormalon dominance picture [14]; $c_3$ differs by less than 3% when we use these estimates, for $n_f = 4, 5$.† We also varied $a_3$ by ±100% in Eq. (2) and find that $c_3$ changes by less than ±10% for $n_f = 4, 5$. As we can see from the table, the large-$\beta_0$ approximation turns out to lie between 85% and 120% of the full result in the relevant cases. We observe that the agreement becomes substantially worse if we remove the log $\alpha_S$ term from the full result.

In Figs. 1a) and b), we show the renormalization scale ($\mu$) dependences of the $1S$ energy level when we use the pole mass and the $\overline{\text{MS}}$ mass‡, respectively, to express the energy level. We used the $\epsilon$-expansion [15] to cancel renormalons in the $\overline{\text{MS}}$ mass scheme; the relevant formulas are given in the Appendix. Fig. 1a) is essentially a reproduction of Fig. 2(b) of [2], by including the leading order (LO) curve in addition. As pointed out by [2], the next-to-next-to-next-to-leading order (NNNLO) prediction becomes insensitive to the scale variation at $\mu \approx 15$ GeV, †The corresponding estimates of the three loop coefficient $a_3$ are given by $a_3(\text{Padé})/4^3 = 98, 60, \text{ and } a_3(\text{Pineda})/4^3 = 72, 37 \text{ for } n_f = 4, 5$, respectively [5, 14].

‡The pole-$\overline{\text{MS}}$ mass relation is known up to 3 loops presently. The 4-loop correction is replaced by its large-$\beta_0$ approximation in our analysis.
Figure 1: The renormalization scale dependences of the energy level of the vector toponium 1S state for a) the pole mass scheme and b) $\overline{\text{MS}}$ mass scheme, respectively. The solid curves are the NNNLO results, dotted, dashed and dot-dashed curves denote the LO, NLO and NNLO results, respectively.

and that the sum of the $\mathcal{O}(\alpha_s^5 m)$ and $\mathcal{O}(\alpha_s^5 m \log \alpha_s)$ corrections becomes small around this scale. On the other hand, in Fig. 1b), we see a good convergence behavior at $\mu \sim 50–80$ GeV. In Fig. 2 the vertical scale is magnified and the scale dependences of the energy levels at the NNNLO in both mass schemes are compared. We find a much better stability of the prediction in the $\overline{\text{MS}}$ mass scheme over a wide region $40 \text{ GeV} < \mu < 160 \text{ GeV}$. From this analysis, we consider the scale $\mu \sim 50–80$ GeV to be an optimal scale choice in the $\overline{\text{MS}}$ mass scheme. By varying $\mu$ between $30–160$ GeV, we estimate the theoretical error of the $\overline{\text{MS}}$ mass to be order $40 \text{ MeV}$ at NNNLO if it is extracted from the 1S energy level. (We obtain an error of about $200 \text{ MeV}$ if a similar estimate is applied for the pole mass.)

In the pole mass scheme, it is natural to choose the renormalization scale around the Bohr scale, $\mu \sim C_F \alpha_s m \sim 30$ GeV. This is because there is only one logarithm $\log(\mu/(C_F \alpha_s m))$ in the energy level, associated with the renormalization scale $\mu$,§ and because this logarithm is minimized around the Bohr scale. On the other hand, in the $\overline{\text{MS}}$ mass scheme, two types of logarithms $\log(\mu/m)$ and $\log(\mu/(C_F \alpha_s m))$ are included in the expression for the energy level,¶ where $m = m_{\overline{\text{MS}}} (m_{\overline{\text{MS}}})$ is the renormalization-group invariant $\overline{\text{MS}}$ mass; see Eqs. (13), (17) and (18). Therefore, a natural scale, which minimizes the logarithmic contributions, lies between the Bohr scale and the hard scale, $C_F \alpha_s m < \mu < m$. This aspect of the renormalization scale, when the leading renormalon uncertainty is removed, has been discussed already for the bottomonium energy levels [16], and a further detailed study of the scale choice (in the context of the QCD potential) has been given in [17].

If we replace $c_3$ by $c_3(\text{large-}\beta_0)$, the corresponding figures to Figs. 1a,b) and 2 look very

§ At NNNLO, the logarithm associated with the ultrasoft scale $\sim \alpha_s^2 m$ is not accompanied by the renormalization scale $\mu$.

¶ This stems from the fact that one needs to expand the pole mass and the binding energy in the same coupling constant $\alpha_s(\mu)$ in order to achieve the decoupling of infrared degrees of freedom at each order of the perturbative expansion.
similar; these were shown in [18]. The main observations in the analysis in the large-$\beta_0$ approximation were as follows [12, 18]: (1) In the pole mass scheme, with any choice of the scale $\mu$, the perturbative series of the $1S$ energy level does not show a healthy convergence behavior, hence the level cannot be predicted with an accuracy better than $\mathcal{O}(\Lambda_{\text{QCD}})$. (2) In the $\overline{\text{MS}}$ mass scheme, one observes a good convergence of the perturbative series in the range $m_\alpha < \mu < m$, as well as stability of the prediction in this range. Both of these observations still hold at the best of our present knowledge. It is intriguing whether these features will remain valid even when $a_3$ and the 4-loop relation between the pole and $\overline{\text{MS}}$ masses are computed fully in the future.

Let us address how the theoretical error of about 80 MeV for the top quark pole mass was obtained in Ref. [2]. It is dominated by the uncertainty induced by the error of the input $\alpha_S(M_Z)$. The uncertainty due to the scale dependence was estimated by varying $\mu$ between 10–30 GeV and an error of $20.5(=41/2)$ MeV was assigned as an uncertainty from this source. Uncertainties from other sources were estimated to be even smaller. Here, let us concentrate on the error estimate from the scale dependence and discuss its problem. The smallness of this error ensures, partly, the smallness of the total error (80 MeV). However, if the same estimation method is applied to the LO and NLO curves in Fig. 1a), we should infer that the NNLO correction is small, in contradiction to its true large size. Thus, apparently there is a danger in relying on this estimation method. By contrast, our error estimate of the top quark $\overline{\text{MS}}$ mass from the scale dependence does not suffer from the same problem. The same estimation method works at lower orders, because the perturbative series in Fig. 1b) shows a healthy convergence behavior and the scale dependence decreases as we include more terms around the relevant scales.

At this stage, there seems to be a puzzling point: on the one hand, the validity of the large-
\[ n = \frac{2\pi}{\beta_0 \alpha_s(\mu)} \]

Figure 3: The graph showing schematically the asymptotic behavior of the \( n \)-th term of \(-E_{1S}\) in the large-\( \beta_0 \) approximation for \( n \gg 1 \).

\[ \beta_0 \text{ approximation is known to lead to an } O(\Lambda_{\text{QCD}}) \text{ uncertainty of the pole mass; on the other hand, the small size of the } O(\alpha^5_S m) \text{ plus } O(\alpha^5_S m \log \alpha_S) \text{ corrections in the range } \mu \sim 10-30 \text{ GeV appears to be incompatible with the renormalon picture.} \]

Let us recall the estimate of the renormalon uncertainty in the large-\( \beta_0 \) approximation (see e.g. [19]). Asymptotically the perturbative series of the \( 1S \) energy level, if expressed in the pole mass, behaves as

\[ E_{1S}(n) \sim \text{const.} \times \mu \alpha_S(\mu) \times \left\{ \frac{\beta_0 \alpha_S(\mu)}{2\pi} \right\}^n \times n! \quad \text{for} \quad n \gg 1. \tag{4} \]

It becomes minimal at \( n \approx n_* \equiv 2\pi/(\beta_0 \alpha_S(\mu)) \). The size of the term scarcely changes within the range \( n \in (n_* - \sqrt{n_*}, n_* + \sqrt{n_*}) \); see Fig. 3.\footnote{Using the Stirling formula, one may easily find an approximate position \( n_* \) of the minimum of the series. Then, by expanding around the minimum, one finds an approximate form \( n! n_*^{-n} \approx \sqrt{2\pi n_*} \exp[-n_* + (n - n_*)^2/(2n_*)] \sim \sqrt{2\pi n_*} \exp(-n_*) \) in the range \( |n - n_*| \ll \sqrt{n_*} \).}

We may consider the uncertainty of this asymptotic series as the sum of the terms within this range, since we are not sure where to truncate the series within this range:

\[ \delta E_{1S} \sim \left| \sum_{n=n_*-\sqrt{n_*}}^{n_*+\sqrt{n_*}} E_{1S}(n) \right| \sim \Lambda_{\text{QCD}}. \tag{5} \]

The \( \mu \)-dependence vanishes in this sum, and this leads to the claimed uncertainty. This argument shows that when the relevant coupling constant \( \alpha_S(\mu) \) is small (corresponding scale \( \mu \) is large), \( n_* \) is large. Then each term of the series for \( n \in (n_* - \sqrt{n_*}, n_* + \sqrt{n_*}) \) can become considerably smaller than \( \Lambda_{\text{QCD}} \).

According to this argument, the small size of the \( O(\alpha^5_S m) \) plus \( O(\alpha^5_S m \log \alpha_S) \) correction at certain scales does not generally lead to an uncertainty considerably smaller than \( \Lambda_{\text{QCD}} \).
While an error estimate should necessarily be more or less subjective, as long as the large-$\beta_0$ approximation is valid, we should at least bear in mind how the theoretical uncertainty is estimated in this framework. Incidentally, based on the large-$\beta_0$ approximation, the $\overline{\text{MS}}$ mass extracted from the $1S$ energy level has an uncertainty of order $\Lambda_{\text{QCD}}^3/\mu^2_{\text{opt}} \sim 3-10$ MeV originating from the next-to-leading order renormalon contribution \[20\]. Thus, the above perturbative error of order 40 MeV is still significantly larger than this contribution.

To conclude, we observe a much more stable prediction of the toponium $1S$ energy level when we use the $\overline{\text{MS}}$ mass instead of the pole mass. Considering this situation and the good agreement of the large-$\beta_0$ approximation with the presently known corrections, we consider a theoretical uncertainty of the pole mass of order $\Lambda_{\text{QCD}} \sim 200-300$ MeV to be legitimate. On the other hand, based on the argument in \[12\], it is likely that the top quark $\overline{\text{MS}}$ mass can be extracted with an accuracy of order 40 MeV, once the 4-loop relation between the pole and $\overline{\text{MS}}$ mass is calculated. This number may be compared with the most recent estimate \[21\] of the experimental error (including some systematic errors) of 19 MeV in the determination of the top quark $1S$ mass, corresponding to a 3-parameter fit with an integrated luminosity of 300 fb$^{-1}$.

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**Appendix**

In this appendix we list the formulas we use to convert the energy level of the quarkonium $1S$ state from the pole mass scheme to the $\overline{\text{MS}}$ mass scheme using the $\varepsilon$-expansion \[15\].

The energy of the quarkonium $1S$ state is given by

$$M_{1S} = 2m_{\text{pole}} + E_{1S}(m_{\text{pole}}, \alpha_S(\mu)) \quad (6)$$

as a function of $m_{\text{pole}}$ and $\alpha_S(\mu) = \alpha_S^{(n_f)}(\mu)$ in the pole mass scheme, where $n_f$ is the number of light quark flavors ($n_f = 4, 5$ for the bottomonium and toponium, respectively). Mass relation between the pole and $\overline{\text{MS}}$ masses is given by

$$m_{\text{pole}} = \overline{m} \left\{ 1 + d_0 \frac{\varepsilon \alpha_S(\overline{m})}{\pi} + d_1 \left( \frac{\varepsilon \alpha_S(\overline{m})}{\pi} \right)^2 + d_2 \left( \frac{\varepsilon \alpha_S(\overline{m})}{\pi} \right)^3 + d_3 \left( \frac{\varepsilon \alpha_S(\overline{m})}{\pi} \right)^4 + O(\varepsilon^5) \right\}, \quad (7)$$

where $\varepsilon = 1$ is the expansion parameter in the $\varepsilon$-expansion, $\overline{m} \equiv m_{\overline{\text{MS}}}(m_{\overline{\text{MS}}})$, $d_0 = 4/3$.

The coefficients $d_1$ and $d_2$ are obtained from the 2-loop \[22\] and 3-loop \[9\] mass relations *.*, *The same relation was obtained numerically before in \[24\] in a certain approximation.*
Using Eqs. (7) and (11), we obtain the

\[ d_1 = \frac{307}{32} + \frac{\pi^2}{3} + \frac{\pi^2 \log 2}{9} - \frac{\zeta_3}{6} + n_f \left( -\frac{71}{144} + \frac{\pi^2}{18} \right) \]

\[ \approx 13.4434 - 1.04137 n_f, \quad (8) \]

\[ d_2 = \frac{8462917}{93312} + \frac{652841 \pi^2}{38880} - \frac{695 \pi^4}{7776} - \frac{575 \pi^2 \log 2}{162} \]

\[ - \frac{22 \pi^2 \log^2 2}{81} - \frac{55 \log^4 2}{162} + \frac{220 \text{Li}_4(\frac{1}{2})}{27} + \frac{58 \zeta_3}{27} - \frac{1439 \pi^2 \zeta_3}{432} + \frac{1975 \zeta_5}{216} \]

\[ + n_f \left( -\frac{231847}{23328} + \frac{991 \pi^2}{648} + \frac{61 \pi^4}{1944} - \frac{11 \pi^2 \log 2}{81} + \frac{2 \pi^2 \log^2 2}{81} \right) \]

\[ + \frac{8 \text{Li}_4(\frac{1}{2})}{27} - \frac{241 \zeta_3}{72} \right) + n_f^2 \left( \frac{2353}{23328} + \frac{13 \pi^2}{324} + \frac{7 \zeta_3}{54} \right) \]

\[ \approx 190.391 - 26.6551 n_f + 0.652691 n_f^2, \quad (9) \]

with \( \zeta_3 = 1.20206 \cdots \), \( \text{Li}_4(\frac{1}{2}) = 0.517479 \cdots \). The third coefficient \( d_3 \) is not known exactly yet. In this paper we use its value in the large-\( \beta_0 \) approximation [7]:

\[ d_3(\text{large-} \beta_0) = \frac{\beta_0^3}{64} \left( \frac{42979}{5184} + \frac{89 \pi^2}{18} + \frac{71 \pi^4}{120} + \frac{317 \zeta_3}{12} \right) \]

\[ \approx 3046.29 - 553.872 n_f + 33.568 n_f^2 - 0.678141 n_f^3. \quad (10) \]

To achieve the renormalon cancellation between \( 2m_{\text{pole}} \) and \( E_{1S}(m_{\text{pole}}, \alpha_S(\mu)) \) order by order in the \( \varepsilon \)-expansion, we must use the same coupling constant \( \alpha_S(\mu) \) in the series expansions of \( 2m_{\text{pole}} \) and \( E_{1S} \). Therefore, \( \alpha_S(\overline{\mu}) \) is re-expressed in terms of \( \alpha_S(\mu) \) as

\[ \alpha_S(\overline{\mu}) = \alpha_S(\mu) \left\{ 1 + \frac{\beta_0 \log(\frac{\mu}{\overline{\mu}})}{2} \left( \varepsilon \alpha_S(\mu) \right) \pi + \left( \frac{\beta_1 \log(\frac{\mu}{\overline{\mu}})}{8} + \frac{\beta_0^2 \log^2(\frac{\mu}{\overline{\mu}})}{4} \right) \left( \frac{\varepsilon \alpha_S(\mu)}{\pi} \right)^2 \right. \]

\[ + \left( \frac{\beta_2 \log^3(\frac{\mu}{\overline{\mu}})}{32} + \frac{5\beta_0 \beta_1 \log^2(\frac{\mu}{\overline{\mu}})}{32} + \frac{\beta_2^3 \log^3(\frac{\mu}{\overline{\mu}})}{8} \right) \left( \frac{\varepsilon \alpha_S(\mu)}{\pi} \right)^3 \right\} + \mathcal{O}(\varepsilon^4), \quad (11) \]

using the coefficients of the QCD \( \beta \)-function:

\[ \beta_0 = 11 - \frac{2 n_f}{3}, \quad \beta_1 = 102 - \frac{38 n_f}{3}, \quad \beta_2 = \frac{2857}{2} - \frac{5033 n_f}{18} + \frac{325 n_f^2}{54}. \quad (12) \]

Using Eqs. (7) and (11), we obtain the \( \varepsilon \)-expansion for \( m_{\text{pole}} \) in terms of \( \alpha_S(\mu) \),

\[ m_{\text{pole}} = \overline{\mu} \times \left( 1 + \sum_{n=1}^{4} \tilde{d}_{n-1}(\mu) \varepsilon^n \left( \frac{\alpha_S(\mu)}{\pi} \right)^n \right) + \mathcal{O}(\varepsilon^5), \quad (13) \]
where the coefficients $\tilde{d}_n(l_\mu)$ are functions of $l_\mu = \log(\mu/\overline{m})$ which enter via Eq. (13).

The binding energy $E_{1S}(m_{\text{pole}}, \alpha_S(\mu))$ is given by

$$E_{1S} = -\frac{4}{9} \alpha_S(\mu)^2 m_{\text{pole}} \sum_{n=0}^\infty \varepsilon^{n+1} \left( \frac{\alpha_S(\mu)}{\pi} \right)^n P_n(L_\mu),$$

(14)

where $L_\mu = \log [\mu/(C_F\alpha_S(\mu)m_{\text{pole}})]$, and $P_n(L_\mu)$ are given by

$$P_0(L_\mu) = 1,$$

$$P_1(L_\mu) = \beta_0 L_\mu + c_1,$$

$$P_2(L_\mu) = \frac{3}{4} \beta_0^3 L_\mu^2 + \left( \frac{1}{2} \beta_0^2 + \frac{1}{4} \beta_1 + \frac{3}{2} \beta_0 c_1 \right) L_\mu + c_2,$$

$$P_3(L_\mu) = \frac{1}{2} \beta_0^3 L_\mu^3 + \left( -\frac{7}{8} \beta_0^3 + \frac{7}{16} \beta_0 \beta_1 + \frac{3}{2} \beta_0^2 c_1 \right) L_\mu^2$$

$$+ \left( \frac{1}{4} \beta_0^3 - \frac{1}{4} \beta_0 \beta_1 + \frac{1}{16} \beta_2 - \frac{3}{4} \beta_0^2 c_1 + \frac{3}{8} \beta_1 c_1 + 2 \beta_0 c_2 \right) L_\mu + c_3,$$

(15)

with

$$c_1 = \frac{97}{6} - \frac{11}{9} n_f,$$

$$c_2 = \frac{1793}{12} + \frac{2917 \pi^2}{216} - \frac{9 \pi^4}{32} + \frac{275 \zeta_3}{4} + \left( -\frac{1693}{72} - \frac{11 \pi^2}{18} - \frac{19 \zeta_3}{2} \right) n_f + \left( \frac{77}{108} + \frac{\pi^2}{54} + \frac{2 \zeta_3}{9} \right) n_f^2.$$

(16)

The terms which contain $L_\mu$ are determined by renormalization-group equation from lower order constants $c_{1,2}$. The $c_{1,2}$ are taken from [23], $c_3$ is given in Eq. (2). To obtain the $\varepsilon$-expansion in the $\overline{\text{MS}}$ scheme, we re-express the pole mass in $E_{1S}(m_{\text{pole}}, \alpha_S(\mu))$ by $\overline{m}$ and $\alpha_S(\mu)$ employing the mass relation Eq. (13), which gives

$$E_{1S} = -\frac{4}{9} \alpha_S(\mu)^2 \overline{m} \sum_{n=0}^3 \varepsilon^{n+1} \left( \frac{\alpha_S(\mu)}{\pi} \right)^n \tilde{P}_n(\overline{L}_\mu, l_\mu), + \mathcal{O}(\varepsilon^5),$$

(17)

with $\tilde{L}_\mu = \log [\mu/(C_F\alpha_S(\mu)\overline{m})]$. Using the $\varepsilon$-expansions Eqs. (13) and (17), $M_{1S}$ is rewritten as

$$M_{1S} = \frac{2\overline{m}}{\alpha_S(\mu)^2} \sum_{n=1}^4 \tilde{d}_{n-1}(l_\mu) \varepsilon^n \left( \frac{\alpha_S(\mu)}{\pi} \right)^n - \frac{4}{9} \alpha_S(\mu)^2 \overline{m} \left( \sum_{n=0}^3 \varepsilon^{n+1} \left( \frac{\alpha_S(\mu)}{\pi} \right)^n \tilde{P}_n(\overline{L}_\mu, l_\mu) \right)$$

$$= \frac{2\overline{m}}{\alpha_S(\mu)} \left[ 1 + \sum_{n=1}^4 \tilde{d}_{n-1}(l_\mu) - \frac{2\pi \alpha_S(\mu)}{9} \tilde{P}_{n-1}(\overline{L}_\mu, l_\mu) \right] \varepsilon^n \left( \frac{\alpha_S(\mu)}{\pi} \right)^n.$$

(18)

Setting the expansion parameter $\varepsilon = 1$ in the final expression, the $n$-th order correction to $M_{1S}$ in the $\overline{\text{MS}}$ scheme is given by $2\overline{m} \times (\alpha_S(\mu)/\pi)^n \left[ \tilde{d}_{n-1}(l_\mu) - (2\pi \alpha_S(\mu)/9) \tilde{P}_{n-1}(\overline{L}_\mu, l_\mu) \right]$.

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