Heavy Quarkonium Spectrum at $\mathcal{O}(\alpha_s^5 m_q)$ and Bottom/Top Quark Mass Determination.

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Abstract

We present the next-to-next-to-next-to-leading $\mathcal{O}(\alpha_s^5 m_q)$ result for the ground state energy of a heavy quarkonium system. On the basis of this result we determine the bottom quark mass from $\Upsilon(1S)$ resonance and provide an explicit formula relating the top quark mass to the resonance energy in $t\bar{t}$ threshold production.

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1 Introduction

Quark masses enter the Lagrangian of Quantum Chromodynamics (QCD) as fundamental parameters. Thus, it is of primary interest to perform accurate determinations of the mass values combining experimental input with precision calculations from the theoretical side. In this letter we focus on the bottom and top quark masses. The bottom quark mass is of particular interest due to the current and future $B$ physics experiments. In the observables used to extract the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements and to gain deeper insight in the understanding of CP violation the bottom quark mass enters as a crucial input quantity. Thus a precise knowledge of the latter is essential for the interpretation of the experimental data. On the other hand, the top quark mass is one of the key parameters for precision tests of the standard model of the electroweak interactions at high energies and for the search of “new physics” at a future $e^+e^-$ linear collider.

Whereas the masses of the up, down and strange quark require major non-perturbative input the higher quark masses can be computed with relatively high accuracy using perturbative methods. The study of nonrelativistic heavy-quark-antiquark systems is one of the most promising approaches in this respect. These systems allow for a model-independent perturbative treatment which relies entirely on first principles of QCD $^1$. Nonperturbative effects $^2,\,^3$ are well under control for the top-antitop system and, at
least for the ground state resonance, also for bottomonium. This makes heavy-quark-
antiquark systems an ideal laboratory to determine the heavy-quark masses. Besides its
phenomenological importance, the heavy-quarkonium system is very interesting from the
theoretical point of view because it possesses a highly sophisticated multiscale dynamics
and its study demands the full power of the effective-theory approach.

Among other characteristics of the heavy quarkonium system the ground state energy
is of primary phenomenological interest. It can be directly used to extract the bottom
quark mass from the lowest resonance of the Υ family and essentially determines the re-
sonance energy in $t\bar{t}$ threshold production. The $O(\alpha_s^4m_q)$ heavy quarkonium spectrum was
obtained first in [4] and afterwards confirmed in [5,6]. At $O(\alpha_s^5m_q)$ the heavy quarkonium
spectrum was derived in [7] for vanishing $\beta$-function and the large-$\beta_0$ result can be found
in [8,9].

In the present letter we complete the result of [7] for the ground state energy by
calculating the remaining terms proportional to $\beta$-function. We apply the result to the
determination of the bottom quark mass from the mass of $\Upsilon(1S)$ resonance and give
an explicit formula relating the top quark mass to the resonance energy in $t\bar{t}$ threshold
production both for $e^+e^-$ annihilation and $\gamma\gamma$ collisions. The main results are given by
Eqs. (12), (18) and (21).

2 Perturbative heavy quarkonium ground state energy at $O(\alpha_s^5m_q)$

For the calculation of the ground state energy we follow the general approach of [4,10].
It is based on the nonrelativistic effective theory concept [11,12] in its potential NRQCD
(pNRQCD) incarnation [13] and is implemented with the threshold expansion [14]. In
pNRQCD the dynamics of the nonrelativistic potential heavy quark-antiquark pair is
governed by the effective Schrödinger equation and by its multipole interaction to the ul-
trasoft gluons. The relativistic effects of the harder modes that have been “integrated out”
are encoded in the higher-dimensional operators which appear in the effective Hamiltonian
and correspond to an expansion in the heavy quark velocity $v$, and the Wilson coefficients
which are series in the strong coupling constant $\alpha_s$.

The analysis of the heavy quarkonium spectrum at $O(\alpha_s^5m_q)$, i.e. the third order
corrections to the Coulomb approximation involves two basic ingredients: the effective
Hamiltonian and the retardation effect associated with the emission and absorption of
dynamical ultrasoft gluons. The general form of the Hamiltonian valid up to next-to-
next-to-leading order$^1$ (N$^3$LO) is given in [15]. A detailed discussion of the effects
resulting from the chromoelectric dipole interaction of the heavy quark-antiquark pair to

$^1$In such a framework one has two expansion parameters, $\alpha_s$ and $v$. The corrections are classified
according to the total power of $\alpha_s$ and $v$, i.e. N$^k$LO corrections contain terms of $O(\alpha_s^l v^m)$, with
$l + m = k$. This has the consequence that, in general, different loop orders, which are counted in
powers of $\alpha_s$, contribute to the N$^k$LO result. Note, that for the corrections to the parameters of a heavy
quarkonium bound state, where $v \sim \alpha_s$, the standard ordering in powers of $\alpha_s$ is restored.
the ultrasoft gluons relevant for perturbative bound-state calculations at $N^3\text{LO}$ can be found in [4].

For vanishing angular momentum we can write the energy level of the principal quantum number $n$ as

$$E_n^{p.t.} = E_n^C + \delta E_n^{(1)} + \delta E_n^{(2)} + \delta E_n^{(3)} + \ldots,$$

where the leading order Coulomb energy is given by

$$E_n^C = -\frac{C^2_F \alpha_s^2 m_q}{4n^2}.$$

$\delta E_n^{(k)}$ stands for corrections of order $\alpha_s^k$. The first and second order corrections can be found in [4,5,6] for arbitrary $n$. For the ground state one gets

$$\delta E_1^{(1)} = E_1^C \frac{\alpha_s}{\pi} \left[ 4\beta_0 L_\mu + 4\beta_0 + \frac{a_1}{2} \right],$$

$$\delta E_1^{(2)} = E_1^C \left( \frac{\alpha_s}{\pi} \right)^2 \left[ 12\beta_0^2 L_\mu^2 + \left( 16\beta_0^2 + 3a_1\beta_0 + 4\beta_1 \right) L_\mu + \left( 4 + \frac{2\pi^2}{3} + 8\zeta(3) \right) \beta_0^2 + 2a_1\beta_0 + 4\beta_1 + \frac{a_2}{16} + \frac{a_3}{8} + \pi^2 C_A C_F + \left( \frac{21\pi^2}{16} - \frac{2\pi^2}{3} S(S+1) \right) C_F^2 \right],$$

where $L_\mu = \ln(\mu/(C_F \alpha_s m_q))$, $\zeta(3) = 1.202057 \ldots$ is Riemann’s $\zeta$-function, $C_F = 4/3$ and $C_A = 3$ are the eigenvalues of the quadratic Casimir operators of the fundamental and adjoint representations of the colour gauge group, respectively. The modified minimal-subtraction (\overline{\text{MS}}) scheme for the renormalization of $\alpha_s$ is implied. The coefficients $a_i$ parameterize the $i$-loop perturbative corrections to the Coulomb potential. The analytical results for the one- [16,17] and two-loop [18,19,10] coefficients are

$$a_1 = \frac{31}{9} C_A - \frac{20}{9} T_F n_l,$$

$$a_2 = \left[ \frac{4343}{162} + 4\pi^2 - \frac{\pi^4}{4} + \frac{22}{3} \zeta(3) \right] C_A^2 - \left[ \frac{1798}{81} + \frac{56}{3} \zeta(3) \right] C_A T_F n_l$$

$$- \left[ \frac{55}{3} - 16\zeta(3) \right] C_F T_F n_l + \left( \frac{20}{9} T_F n_l \right)^2,$$

where $T_F = 1/2$ is the index of the fundamental representation and $n_l$ is the number of light-quark flavors. For convenience of the reader we also provide the first three coefficients of the QCD $\beta$-function

$$\beta_0 = \frac{1}{4} \left( \frac{11}{3} C_A - \frac{4}{3} T_F n_l \right),$$

$$\beta_1 = \frac{1}{16} \left( \frac{34}{3} C_A^2 - \frac{20}{3} C_A T_F n_l - 4C_F T_F n_l \right),$$

$$\beta_2 = \frac{1}{64} \left( \frac{2857}{54} C_A^3 - \frac{1415}{27} C_A^2 T_F n_l - \frac{205}{9} C_A C_F T_F n_l + 2C_F^2 T_F n_l + \frac{158}{27} C_A T_F^2 n_l^2 \right.$$

$$+ \frac{44}{9} C_F T_F^2 n_l^2 \right).$$

(5)
The $\mathcal{O}(\alpha_s^3)$ corrections to the energy levels arise from several sources:

(i) matrix elements of the N$^3$LO operators of the effective Hamiltonian between Coulomb wave functions;

(ii) higher iterations of the NLO and NNLO operators of the effective Hamiltonian in time-independent perturbation theory;

(iii) matrix elements of the N$^3$LO instantaneous operators generated by the emission and absorption of ultrasoft gluons; and

(iv) the retarded ultrasoft contribution.

The contributions to $E^{(3)}_n$ for vanishing $\beta$-function were computed for general $n$ in [7]. The corresponding correction to the ground state energy gets contributions from all four sources and reads

$$\delta E^{(3)}_1 |_{\beta(\alpha_s) = 0} = -E^C_1 \frac{\alpha_s^3}{\pi} \left\{ -\frac{a_1 a_2 + a_3}{32 \pi^2} + \left[ -\frac{C_A C_F}{2} + \left( \frac{-11}{16} + \frac{S(S+1)}{2} \right) C_F^2 \right] a_1 \right. $$

\[ + \left[ \frac{1}{36} + \ln \frac{2}{6} + \frac{L_{\alpha_s}}{6} \right] C_A^3 + \left[ -\frac{49}{36} + \frac{4}{3} \left( \ln 2 + L_{\alpha_s} \right) \right] C_A^2 C_F^2 \]

\[ + \left[ \frac{5}{72} + \frac{10}{3} \ln 2 + \frac{37}{6} L_{\alpha_s} + \left( \frac{85}{54} - \frac{7}{6} L_{\alpha_s} \right) S(S+1) \right] C_F^3 \]

\[ + \left[ \frac{50}{9} + \frac{8}{3} \ln 2 + 3 L_{\alpha_s} - \frac{S(S+1)}{3} \right] C_F^2 T_F \]

\[ + \left[ \frac{32}{15} + 2 \ln 2 + (1 - \ln 2) S(S+1) \right] C_F^2 T_F n_t \]

\[ + \left[ \frac{11}{18} - \frac{10}{27} S(S+1) \right] C_F^2 T_F n_l + \frac{2}{3} C_F L^E_1 \right\}, \quad (6) \]

where $S$ is the spin quantum number and $L_{\alpha_s} = -\ln(C_F \alpha_s)$. The terms proportional to $a_1$ correspond to the iterations of lower-order operators as mentioned in point (ii) of the above list. The last term in Eq. (6) corresponds to retarded ultrasoft contribution (cf. point (iv)). The corresponding QCD Bethe logarithms can be found in [15,7] with the numerical result $L^E_1 = -81.5379$. The logarithmic $\ln(\alpha_s)$ part of Eq. (6) is known from previous analyses [20,21]. At present, only Padé estimates of the three-loop MS coefficient $a_3$ are available [22]. For the bottom and top quark case they read

$$a_3 \left\{ \begin{array}{ll} 98 & \text{if } n_l = 4, \\ 60 & \text{if } n_l = 5. \end{array} \right. \quad (7) $$

Note that at N$^3$LO the Wilson coefficients in the effective Hamiltonian are infrared (IR) divergent. The corresponding divergence is canceled against the ultraviolet (UV) one of the ultrasoft contribution. In our analysis based on the threshold expansion dimensional regularization is used to handle the divergences. For convenience, the IR singular pole
part of the Wilson coefficients is subtracted according to the $\overline{\text{MS}}$ prescription, so that the coefficients, in particular $a_3$, are defined in the $\overline{\text{MS}}$ subtraction scheme both for UV and IR divergences. For consistency, the UV pole of the ultrasoft contribution is subtracted in the same way [7].

The third order corrections to the ground state energy proportional to the $\beta$-function only get contributions from (i) and (ii). The computation of the contribution from (i) is rather straightforward. It includes the corrections due to the three-loop running of the Coulomb potential which we mark by $C.r.$, and the one-loop running of the $1/m_q$ suppressed and the Breit potential ($B.r.$) of the following form

\[
\delta E^{(3)}_{C.r.} = E_1^{C_r} \left( \frac{\alpha_s}{\pi} \right)^3 \left( 16\beta_0^3 L_\mu^3 + \left[ 48\beta_0^3 + 6a_1\beta_0^2 + 20\beta_1\beta_0 \right] L_\mu^2 \\
+ \left[ 12\pi^2 \beta_0^3 + 12a_1\beta_0^2 + \left( 40\beta_1 + \frac{3}{4}a_2 \right) \beta_0 + 2a_1\beta_1 + 4\beta_2 \right] L_\mu \\
+ 12\pi^2 \beta_0^3 + \frac{3\pi^2}{2} a_1\beta_0^2 + \left( 5\pi^2 \beta_1 + \frac{3}{4}a_2 \right) \beta_0 + 2a_1\beta_1 + 4\beta_2 \right) \right], \quad (8)
\]

\[
\delta E^{(3)}_{B.r.} = E_1^{C_r} \left( \frac{\alpha_s}{\pi} \right)^3 \left\{ \left[ 4C_A C_F + \left( 1 - \frac{4S(S+1)}{3} \right) C_F^2 \right] L_\mu \\
+ \left( -1 + \frac{4S(S+1)}{3} \right) C_F^2 \right\}. \quad (9)
\]

The contribution of the type (ii) can be computed using the general approach of [6,23] (see also [8]). It includes the corrections due to the iterations of the one- and two-loop running of the Coulomb potential which we mark by $C.i.$, and the iteration of the kinetic energy correction, the $1/m_q$ and the Breit potential with the one-loop running of the Coulomb potential ($B.i.$). The corresponding analytical expressions read

\[
\delta E^{(3)}_{C.i.} = E_1^{C_i} \left( \frac{\alpha_s}{\pi} \right)^3 \left\{ 16\beta_0^3 L_\mu^3 + \left[ -8\beta_0^3 + 6a_1\beta_0^2 + 8\beta_1\beta_0 \right] L_\mu \\
+ \left[ \left( -\frac{20\pi^2}{3} + 64\zeta(3) \right) \beta_0^3 - 2a_1\beta_0^2 + \left( \frac{a_1^2}{2} + \frac{a_2}{4} \right) \beta_0 + a_1\beta_1 \right] L_\mu \\
+ \left( -8 - 8\pi^2 + \frac{2\pi^4}{45} + 64\zeta(3) - 8\pi^2\zeta(3) + 96\zeta(5) \right) \beta_0^3 \\
+ \left( -\frac{5\pi^2}{6} + 8\zeta(3) \right) a_1\beta_0^2 + \left( 8 - \frac{8\pi^2}{3} + 16\zeta(3) \right) \beta_1 - \frac{a_1^2}{8} \right\}, \quad (10)
\]

\[
\delta E^{(3)}_{B.i.} = E_1^{C_i} \left( \frac{\alpha_s}{\pi} \right)^3 \left\{ \left[ 4C_A C_F + \left( \frac{19}{2} - 4S(S+1) \right) C_F^2 \right] L_\mu \\
+ \left( 6 - \frac{2\pi^2}{3} \right) C_A C_F + \left( 9 - \frac{4\pi^2}{3} + \left( -\frac{8}{3} + \frac{4\pi^2}{9} \right) S(S+1) \right) C_F^2 \right\}, \quad (11)
\]

where $\zeta(5) = 1.036928 \ldots$. As a cross-check to our analytical calculation we computed the non-trivial ingredients by solving the eigenvalue problem numerically in the limit $\alpha_s \to 0$ with the help of the program `schroedinger.nb` [24].
By adding (8), (9), (10) and (11) we obtain the third order correction to the ground state energy proportional to the $\beta$-function

$$\delta E_{1}^{(3)}|_{\beta(\alpha_s)} = E_{1}^{C} \left( \frac{\alpha_s}{\pi} \right)^{3} \left\{ 32 \beta_{0}^{3} L_{\mu}^{3} + \left[ 40 \beta_{0}^{3} + 12 a_{1} \beta_{0}^{2} + 28 \beta_{1} \beta_{0} \right] L_{\mu}^{2} \right. $$

$$+ \left[ \left( \frac{16\pi^{2}}{3} + 64 \zeta(3) \right) \beta_{0}^{3} + 10 a_{1} \beta_{0}^{2} + \left( 40 \beta_{1} + \frac{a_{1}^{2}}{2} + a_{2} \right) \right. $$

$$+ 8\pi^{2} C_{A} C_{F} + \left( \frac{21\pi^{2}}{2} - \frac{16\pi^{2}}{3} S(S + 1) \right) C_{F}^{2} \beta_{0} + 3 a_{1} \beta_{1} + 4 \beta_{2} \right\} L_{\mu}^{0} \right.$$ 

$$+ \left( -8 + 4\pi^{2} + \frac{2\pi^{4}}{45} + 64 \zeta(3) - 8\pi^{2} \zeta(3) + 96 \zeta(5) \right) \beta_{0}^{3} + \left( \frac{2\pi^{2}}{3} + 8 \zeta(3) \right) a_{1} \beta_{0}^{2} \right.$$ 

$$+ \left( 8 + \frac{7\pi^{2}}{3} + 16 \zeta(3) \right) \beta_{1} - \frac{a_{1}^{2}}{8} + \frac{3}{4} a_{2} + \left( 6\pi^{2} - \frac{2\pi^{4}}{3} \right) C_{A} C_{F} $$

$$+ \left( 8\pi^{2} - \frac{4\pi^{4}}{3} + \left( - \frac{4\pi^{2}}{3} + \frac{4\pi^{4}}{9} \right) S(S + 1) \right) C_{F}^{2} \beta_{0} + 2 a_{1} \beta_{1} + 4 \beta_{2} \right\}. \quad (12)$$

The terms proportional to $\beta_{3}^{0}$ in Eqs. (12) can be found in [8,9].

The total result for the third order correction to the ground state energy is given by the sum of Eqs. (6) and (12)

$$\delta E_{1}^{(3)} = \delta E_{1}^{(3)}|_{\beta(\alpha_s)=0} + \delta E_{1}^{(3)}|_{\beta(\alpha_s)}. \quad (13)$$

Adopting the choice $\mu_{s} = C_{F} \alpha_{s}(\mu_{s}) m_{q}$ one obtains for the bottom and top system (for $S=1$) in numerical form

$$\delta E_{1}^{(3)} = \alpha_{s}^{3}(\mu_{s}) E_{1}^{C} \left[ \left( 70.590 |_{n=4} \right) + 15.297 \ln(\alpha_{s}(\mu_{s})) + 0.001 a_{3} + \left( 34.229 |_{n=4} \right) \right], \quad (14)$$

where we have separated the contributions arising from $a_{3}$ and $\beta_{3}^{0}$. The only unknown ingredient in our result for $\delta E_{1}^{(3)}$ is the three-loop $\overline{\text{MS}}$ coefficient $a_{3}$ of the corrections to the static potential entering Eq. (3). Up to now there are only estimates based on Padé approximation which we will use in our analysis. However, we will show that our final result only changes marginally even for a rather large deviations of $a_{3}$ from its Padé estimate.

### 3 Bottom and top quark mass determination

In this section we focus on the bottom and top quark mass determination. We fix the value of the strong coupling constant which enters our theoretical expression to $\alpha_{s}^{(5)}(M_{Z}) = 0.1185 \pm 0.002$ [25].
**Bottom quark.** The starting point for the determination of the bottom quark mass is its relation to the mass of the Υ(1S) resonance

\[ M_{\Upsilon(1S)} = 2m_b + E_1^{p.t.} + \delta^{n.p.}E_1, \]

with \( M_{\Upsilon(1S)} = 9.46030(26) \text{ GeV} \). Here \( \delta^{n.p.}E_1 \) is the nonperturbative correction to the ground state energy. The dominant nonperturbative correction is associated with the gluon condensate contribution given by \( \delta^{n.p.}E_1 = 1872^{1275} \text{ MeV} \). For the numerical estimate we use \( \alpha_s^{(4)}(\mu) = 0.304 \) corresponding to the soft normalization scale \( \mu_s = C_F\alpha_s(\mu_s)m_b \) characteristic to the Coulomb problem and \( m_b = 4.83 \text{ GeV} \) which is obtained from Eq. (15) neglecting the corrections to the Coulomb binding energy. This is consistent with neglecting the perturbative correction to Eq. (15). For the gluon condensate we adopt the value from \( \langle \alpha_s G_{\mu\nu}^a G_{\mu\nu}^a \rangle = 0.04(2) \text{ GeV}^4 \). The effect of higher dimension condensates on the ground state energy is small \([26]\). Note, however, that the contribution of the gluon condensate to the energy level of principal quantum number \( n \) grows as \( n^6 \) and becomes unacceptably large already for \( n = 2 \). Thus the excited levels are very sensitive to the nonperturbative long-wave vacuum fluctuations of the gluon field and cannot be used for reliable predictions.

Combining Eq. (15) with the result of the previous section for the perturbative ground state energy up to \( O(m_q\alpha_s^5) \) we obtain the bottom quark mass as a function the renormalization scale of the strong coupling constant normalization, \( \mu \), which is plotted in Fig. 1(a). For the numerical evaluation we extract \( \alpha_s^{(4)}(m_b) \) with \( m_b = 4.83 \text{ GeV} \) from its value at \( M_Z \) using four-loop \( \beta \)-function accompanied with three-loop matching\( \alpha_s^{(4)}(m_b) \) is used as starting point in order to evaluate \( \alpha_s^{(4)}(\mu) \) at N\( k \)-LO with the help of the \( k \)-loop \( \beta \) function. From Fig. 1(a) we see that the dependence on the renormalization scale becomes very strong below \( \mu \sim 2 \text{ GeV} \) which indicates that the perturbative corrections are not under control. However, even above this scale the perturbative series for the pole mass shows no sign of convergence. This means that one can assign a numerical value to the pole mass only in a specified order of perturbation theory.

On the contrary, it is widely believed that the \( \overline{\text{MS}} \) mass \( \overline{m}_b(\mu) \) at the scale \( \mu = \overline{m}_b(\mu) \) is a short-distance object which has much better perturbative properties. Thus, it seems to be reasonable to convert our result for the pole mass into \( \overline{m}_b(\overline{m}_b) \). The relation between \( m_b \) and \( \overline{m}_b(\overline{m}_b) \) is known up to three-loop approximation \([29,30,31]\) and shows sizable perturbative corrections. For this reason we suggest the following procedure to take into account these corrections in a most accurate way. The idea is that from the one-parametric family of \( \overline{m}_b(\mu) \) we can choose a representative corresponding to some scale \( \mu^* \) in such a way that

\[ \overline{m}_b(\mu^*) = m_b. \]  

\(^2\)We use the package RunDec\([28]\) to perform the running and matching of \( \alpha_s \).
For a given fixed-order value of the pole mass Eq. (17) can be solved for $\mu^*$. In particular, for a pole mass to $N^k$LO we use the $k$-loop relation between the $\overline{\text{MS}}$ and pole mass in Eq. (17). Afterwards $m_b(\mu_b^\star)$ can be computed from $m_b(\mu^*)$ solving the RG equation. The advantage of this approach is obvious: we use the finite order relation between $\overline{\text{MS}}$ and pole mass at the scale where they are perturbatively close while the large difference between $\overline{m}_b(\overline{m}_b)$ and $m_b$ is completely covered by the RG evolution which can be computed with very high accuracy as the corresponding anomalous dimension is known to four-loop approximation [32,33]. The only restriction on the method could be connected to the value of $\mu^\star$. It should be large enough to allow for a reliable use of the RG equation. As we will see this condition is satisfied in practice.

In Fig. 1(b) our result for $\overline{m}_b(\overline{m}_b)$ is plotted at NLO, NNLO and $N^3$LO as a function of the normalization scale $\mu$ which is used to obtain the pole mass $m_b$ (cf. Fig. 1(a)). It is remarkable that close to $\mu = 2.7$ GeV, which is consistent with the physically motivated soft scale $\mu_s \approx 2$ GeV, both the second and the third order corrections vanish. This fact is a rather strong indication of the convergence of the series for $\overline{m}_b(\overline{m}_b)$. The numerical values for $m_b$, $\overline{m}_b(\overline{m}_b)$ at $\mu = 2.7$ GeV as well as the values of $\mu^\star$ and $\alpha_s(4)(\mu^*)$ are listed in Tab. 1 for the different orders.

An alternative approach to extract $m_b(\mu_b)$ was suggested in [34] within the so-called upsilon-expansion. The basic idea is to correlate the approximation for the energy spectrum and the one of the quark mass relation by matching the leading powers of $\beta_0$. As a consequence the $k$th-order correction to the spectrum goes along with the $(k+1)$-loop mass relation. In this way the large corrections proportional to leading powers of $\beta_0$, which are associated to the IR renormalon contribution, are canceled in $\overline{m}_b(\overline{m}_b)$. In order to perform the analysis at $N^3$LO the four-loop relation between the $\overline{\text{MS}}$ and pole mass is necessary for which we adopt the large-$\beta_0$ approximation result [35,9]. One can expect that it is close to the exact answer as the large-$\beta_0$ approximation also works well at three-loop order [29,30]. Adopting this prescription we obtain $\overline{m}_b(\overline{m}_b)$ as shown in Fig. 1(c). Note that within the upsilon-expansion the “scale of best convergence” is absent. Though the NNLO correction vanishes at $\mu \approx 2.7$ GeV as it does within our $\mu^\star$ prescription the $N^3$LO one at this point is sizable as can be seen from Tab. 1. This fact can be explained by the observation that the hypothesis of the renormalon contribution dominance in the perturbative series for the energy levels does not work at $N^3$LO. To be precise, if one sets $\mu = \mu_s$ in Eq. (12) one finds that the renormalon induced term proportional to $\beta_0^3$ is indeed large, however, it covers less than a half of the total third order contribution to $E_1$ which can be seen from Eq. (14). As a consequence, one would have to assign a larger uncertainty from the unknown higher order corrections to the $N^3$LO value given in the last row of Tab. 1.

The uncertainty in the obtained value of $\overline{m}_b(\overline{m}_b)$ originates from several sources which are listed in Tab. 2. Beside the uncertainties in $\alpha_s(5)(M_Z)$ and the gluon condensate one has to take into account the errors in the Padé estimates of the coefficient $a_3$, the charm quark mass effects and the higher order contributions. Let us consider the corresponding errors in more detail. In the above analysis we neglected the charm quark mass both in the correction to the spectrum and in $\overline{\text{MS}}$-pole mass relation. As an estimate of the
Figure 1: (a) Bottom quark pole mass, $m_b$, as a function of the renormalization scale $\mu$, used for the numerical evaluation of $E_1$ where the short-dashed, long-dashed and solid line corresponds to the NLO, NNLO and N$^3$LO approximations. (b) $\overline{\text{MS}}$ bottom quark mass $\overline{m}_b(\overline{m}_b)$, as a function of the renormalization scale $\mu$, which is used for the extraction of the pole mass $m_b$ (cf. (a)). For the conversion from the pole to the $\overline{\text{MS}}$ mass the method described around Eq. (17) is used. (c) like (b), however, the upsilon-expansion is used.
induced error we use the available results incorporating the charm quark mass effects in the spectrum \[ \text{\cite{36,9}} \] and the quark mass relation \[ \text{\cite{37,9}} \]. The value of higher order contributions is difficult to estimate. The nice convergence of the series for \( \overline{m}_b(m_b) \) in the first three orders implies their small size. Commonly the uncertainties from the higher orders are related to the uncertainty induced by a variation of the normalization scale \( \mu \).

We estimate it by allowing a variation of \( \mu \) by \( \pm 400 \text{ MeV} \), which corresponds to twice the difference between the scales at which the NNLO and \( \text{N}^3\text{LO} \) corrections vanish, around our optimal value \( \mu = 2.7 \text{ GeV} \). The uncertainty related to the error in the Padé estimate for \( a_3 \) can be written as \( (a_3^{(n_l=4)}/98 - 1) \times 10 \text{ MeV} \) and will completely disappear once the exact computation becomes available. For the numerical estimate we allow for a \( \pm 100\% \) deviation of \( a_3 \) from the Padé estimate.

Finally, our prediction for the bottom quark \( \overline{\text{MS}} \) mass reads

\[
\overline{m}_b(\overline{m}_b) = 4.346 \pm 0.070 \text{ GeV},
\]

where the uncertainties are added up in quadrature.

Now we are in the position to compare our result to the estimates obtained with other methods. There are different approaches to determine the bottom quark mass from the \( b\bar{b} \) pair production close to threshold which are quite complementary as they are based on different experimental and theoretical input. Three basic techniques can be distinguished:

(i) the direct analysis of the \( \Upsilon \) resonances spectrum;

(ii) low-order moments sum rules;

(iii) the nonrelativistic \( \Upsilon \) sum rules.

Each approach has its own advantages and shortcomings. They are briefly characterized below and the results of the most recent theoretical analyses based on (i) – (iii) are listed in Tab. 3.

The direct analysis of the spectrum of \( \Upsilon \) resonances \[ \text{\cite{1}} \] used in this letter suffers from large nonperturbative corrections. The exited levels are too sensitive to the nonperturbative dynamics and only the ground state can be used for reliable predictions. On the
other hand currently the most accurate perturbative description has been achieved within this framework.

Study of the low-order moments of the spectral density within the sum rules approach relies on the global quark-hadron duality. Nonperturbative effects are negligible. The theoretical analysis consists in fully relativistic fixed-order calculations which have been performed up to NNLO [38]. The method allows for a direct determination of the \( \overline{\text{MS}} \) mass. It is, however, sensitive to the behaviour of the spectral density above the threshold which is not well known experimentally.

The nonrelativistic \( \Upsilon \) sum rules [39] are "between" the approaches (i) and (ii). They operate with the high (of the order \( 1/\alpha_s^2 \)) moments of the spectral density, which are saturated by the nonrelativistic near-threshold region. The experimental input is given by the parameters of the \( \Upsilon \) resonances which are known with high accuracy. On the theoretical side the nonperturbative effects are well under control, however, the Coulomb effects should be properly taken into account. By now the analysis has been performed up to NNLO [40,6,5,41,9]. The extension to \( N^3 \)LO is a challenging theoretical problem. In particular, it requires the calculation of third order corrections to the heavy quarkonium wave function at the origin. The first steps in this direction has been performed in [7,15,21,42,43].

As we see from the Tab. 3 the results of all approaches are in reasonable agreement.

**Top quark.** Let us now turn to the top quark case where the experimental data are not yet available. Our goal is to present a formula which can be directly used for the top quark mass determination from the characteristics of the cross section of \( t \bar{t} \) production near threshold. One has to distinguish the production in \( e^+e^- \) annihilation where the final state quark-antiquark pair is produced with \( S = 1 \) and in (unpolarized) \( \gamma \gamma \) collisions where the dominant contribution is given by the \( S \)-wave zero spin final state.

The nonperturbative effects in the case of the top quark are negligible, however, the

| source | \( \delta \overline{m}_b(\overline{m}_b) \) (MeV) | \( \delta E_{\text{res}} \) (MeV) |
|--------|---------------------------------|------------------|
| \( \alpha_s(M_Z) \) | +13                             | +149             |
| | -8                             | -156             |
| \( \mu \)            | +66                             | ±41              |
| | -47                             |                |
| \( a_3 \)       | ±10                             | ±22              |
| \( \langle GG \rangle \) | ±15                             | -                |
| \( m_c \)         | ±10                             | -                |
| \( \delta^{\Gamma_1}E_{\text{res}} \) | -                             | ±10              |
| total           | ±70                             | ±163             |

Table 2: The sources of uncertainties and corresponding errors in the bottom quark \( \overline{\text{MS}} \) mass and the resonance energy in \( t \bar{t} \) threshold production. The intervals of the input parameters variation are specified in the text. The total uncertainty is obtained by adding up the individual ones in quadrature where in the case of asymmetric errors the maximum is chosen.
Table 3: Recent results for the $\overline{\text{MS}}$ mass obtained in different approaches and approximations.

effect of the top quark width has to be taken into account properly \cite{45} as the relatively large width smears out the Coulomb-like resonances below the threshold. The NNLO analysis of the cross section \cite{46} shows that only the ground state pole results in the well-pronounced resonance. The higher poles and continuum, however, affect the position of the resonance peak and move it to higher energy. As a consequence, the resonance energy can be written in the form

$$E_{\text{res}} = 2m_t + E_t^{\text{p.t.}} + \delta T_E E_{\text{res}}.$$  \hspace{1cm} (19)

To compute the shift of the peak position due to the nonzero top quark width $\delta T_E E_{\text{res}}$ we use the result of \cite{23} for the $e^+e^-\rightarrow t\bar{t}$ and $\gamma\gamma \rightarrow t\bar{t}$ cross sections at NNLO. Numerically we get for both processes

$$\delta T_E E_{\text{res}} = 100 \pm 10 \text{ MeV}. \hspace{1cm} (20)$$

This value is rather stable with respect to the variation of all input parameters of our analysis such as the top quark mass and width, the value of the strong coupling constant and its renormalization scale. In the following we adopt as our central input value $\Gamma_t = 1.43 \text{ GeV} \cite{25}$ and use for the soft renormalization scale $\mu_s = C_F\alpha_s(\mu_s)m_t$. For $m_t = 174.3 \text{ GeV} \cite{25}$ the latter gives $\mu_s \approx 30 \text{ GeV}$.

To evaluate the perturbative contribution we use the result of the previous section up to $N^3\text{LO}$. In Figs. 2(a) and (b) the perturbative ground state energy in NLO, NNLO and $N^3\text{LO}$ is plotted as a function of the renormalization scale of the strong coupling constant for $S = 0$ and $S = 1$, respectively. One can see, that the $N^3\text{LO}$ result shows a much weaker dependence on $\mu$ than the NNLO one. Moreover at the scale $\mu \approx 15 \text{ GeV}$ for $S = 1$ and $\mu \approx 18 \text{ GeV}$ for $S = 0$, which are close to the physically motivated scale $\mu_s$, the $N^3\text{LO}$ correction vanishes and furthermore becomes independent of $\mu$, i.e. the $N^3\text{LO}$ curve shows a local minimum. This suggests the convergence of the series for the ground state energy in the pole mass scheme, which is inconsistent with the renomalon picture. Transforming the result to the $\overline{\text{MS}}$ top quark mass leads to a worse convergence of the series for the resonance energy. However, the difference in the series behaviour due to the use of different mass parameters is less significant than in the case of the bottom quark mass.
Figure 2: Ground state energy $E_{1}^{p.t.}$ of the $t\bar{t}$ bound state in the zero-width approximation as a function of the renormalization scale $\mu$ for $S = 0$ (a) and $S = 1$ (b). The short-dashed, long-dashed and solid line corresponds to the NLO, NNLO and N$^3$LO approximations.

Collecting all the contributions we obtain a universal relation between the resonance energy in $t\bar{t}$ threshold production in $e^+e^-$ annihilation or $\gamma\gamma$ collisions and the top quark pole mass

$$E_{\text{res}} = (1.9833 + 0.007 \frac{m_t - 174.3 \text{ GeV}}{174.3 \text{ GeV}} \pm 0.0009) \times m_t,$$

where the weak nonlinear dependence of Eq. (19) on $m_t$ is taken into account in the second term on the right-hand side of Eq. (21). The central value is computed for $m_t = 174.3$ GeV. The sources of the theoretical uncertainty in Eq. (21) are listed in Tab. 2 in terms of the resonance energy. For the estimates we assume a $\pm 100\%$ error in the Padé approximation of the coefficient $a_3$ and vary the normalization scale in the stability interval which is roughly given by $0.4\mu_s < \mu < \mu_s$. Due to the very nice behaviour of the

...
perturbative expansion for the ground state energy we do not expect large higher order corrections to our result.

4 Conclusions

In this letter we have completed the result of [7] for the N^3LO corrections to the ground state energy of perturbative heavy quarkonium by computing the contributions proportional to the β-function, Eq. (12). We have found that the N^3LO corrections are dominated neither by logarithmically enhanced α_s^3 ln(α_s) nor by the renormalon induced β_0^3 α_s^3 terms (cf. Eq. (14)) and thus the full calculation of the correction is crucial for quantitative analysis.

The result has been applied to determine the bottom quark mass from the mass of the Υ(1S) resonance. The perturbative series for the extracted bottom quark pole mass diverges and should be removed from the analysis in favour of the short-distance mass m_0( m_b) to get a reliable prediction. Our result (18) for m_b( m_b) is in reasonable agreement with the NNLO estimates obtained in the framework of nonrelativistic Υ sum rules and the approach based on low moments, however, with a slightly higher central value.

The explicit formula (21) relating the top quark mass to the resonance energy in t\bar{t} threshold production both in e^+e^- annihilation and γγ collisions has been derived. In contrast to the bottom quark case the perturbative expansion for the ground state energy of a (hypothetical) top-antitop bound state converges very well in the pole mass scheme. As a consequence the top quark pole mass can be extracted from the future experimental data on t\bar{t} threshold production with the theoretical uncertainty of ±80 MeV.

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