Corrections of order $\beta_0^3\alpha_s^3$ to the energy levels and wave function

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One of the most important tasks of a future linear collider is the precise measurement of the threshold production cross section of top quark pairs. In order to match the expected experimental precision it is necessary to perform theoretical predictions which include corrections up to third order in perturbation theory. In this contribution we report about the corrections of order $\beta_0^3\alpha_s^3$ to the heavy quark spectrum and wave function. Physical applications both for the top and bottom quark system are discussed.

1. Motivation

A future linear collider running at a center-of-mass energy close to the production threshold of a top quark pair allows for a precise determination of the mass and width of the top quark, the strong coupling and — in case the Higgs boson is not too heavy — also of the top quark Yukawa coupling. In order to match the expected experimental precision [1] it is important to compute higher-order quantum corrections to this process. In this context we refer to the Refs. [2–6].

The ground state energy to the heavy quarkonium system has been computed in Ref. [3, 4] through $\mathcal{O}(\alpha_s^5 m_q)$ including the third-order correction to the Coulomb approximation. The result has been used to extract m_b from the $\Upsilon(1S)$ meson mass and to derive a formula which relates the top quark mass to the maximum of the cross section below the nominal threshold. The properties of the excited states are more sensitive to the nonperturbative phenomena, and the corresponding perturbative estimates cannot be used, *e.g.*, for the accurate determination of the heavy-quark mass by direct comparison to the meson masses. However, they have to be taken into account in the framework of the nonrelativistic sum rules [7] which is based on the concept of quark-hadron duality and keeps the nonperturbative effects under control. For the practical analysis only a few states with small principal quantum numbers n and zero orbital momentum l are of interest.

A further interesting aspect of investigating the excited states with reliable perturbative results at hand is the possibility to test the effects and structure of the nonperturbative QCD vacuum.

In this contribution we report about the corrections of order $\beta_0^3\alpha_s^3$ to the energy levels for $n = 1, 2$ and 3 [8, 9]. In combination with Ref. [4] this leads to complete third-order results for the energy levels.

As far as the wave function at the origin is concerned a complete result is only available through $\mathcal{O}(\alpha_s^2)$ [10, 11]. The $\mathcal{O}(\alpha_s^2)$ correction has turned out to be so sizeable that the application of perturbation theory for a system of two heavy quarks seemed to be questionable — even for top quarks. Thus it is indispensable to gain full control over the next order. Logarithmically enhanced contributions of order $\mathcal{O}(\alpha_s^3\ln^2\alpha_s)$ and $\mathcal{O}(\alpha_s^3\ln\alpha_s)$ have been computed in Refs. [12, 13] and [5, 6], respectively. In Refs. [8, 9] the next step has been taken and contributions of order $\beta_0^3\alpha_s^3$ have been evaluated. Due to the large numerical value of β_0 these corrections are supposed to be numerically dominant.

2. Energy levels and wave functions to $\mathcal{O}(\beta_0^3\alpha_s^3)$

In the framework of nonrelativistic effective theory [14–17] the corrections to the heavy quarkonium parameters are obtained by evaluating the corrections to the Green function of the effective Schrödinger equation [3]. The β_0^3 part of the third-order contribution, which is the main purpose of this contribution, results from the leading renormalization group running of the static potential, $V_C(r)$. The coordinate space representation of V_C can, e.g., be found in Ref. [8]. At n^{th} order it contains β_0^i terms ($i = 1, \ldots, n$) which are accompanied by logarithms $\ln(\mu r)$ raised to power $1, \ldots, i$.

At third order in perturbation theory one has to consider single iterations of the β_0^3 term, double iterations of the β_0^2 and β_0 term and triple iterations of the first-order corrections proportional to β_0. For the practical computation we use the method elaborated in Refs. [10, 18, 19]. In this way we obtain the corrections to the energy levels and wave function at the origin in the form of multiple harmonic sums. For general n the result is rather cumbersome. However, for a specific n the summation can be performed analytically.

As already mentioned in the Introduction, for practical purpose in the context of sum rules it is certainly sufficient to have results for $n = 1,\ 2,\ 3$ and $l = 0$. For this reason, in Ref. [8] the analytical results have been presented for these values. In Ref. [9] a more general formula has been derived, which however still contains unevaluated sums. After specifying n the same results as in Ref. [8] are obtained.

Let us for completeness present the new results. For vanishing angular momentum the perturbative part of the energy level with principal quantum number n can be written as

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

where $\delta E_n^{(k)}$ stands for corrections of order α_s^k and the leading order Coulomb energy is given by $E_n^C = -C_F^2\alpha_s^2 m_q/(4n^2)$. For the $\mathcal{O}(\beta_0^3\alpha_s^3)$ term we obtain

$$\begin{aligned}
\delta^{(3)}_{\beta_0^3}E_1 &= E_1^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[32L_1^3+40L_1^2+\left(\frac{16\pi^2}{3}+64\zeta(3)\right)L_1-8+4\pi^2+\frac{2\pi^4}{45}+64\zeta(3)-8\pi^2\zeta(3)+96\zeta(5)\right],\\
\delta^{(3)}_{\beta_0^3}E_2 &= E_2^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[32L_2^3+88L_2^2+\left(32+\frac{16\pi^2}{3}+128\zeta(3)\right)L_2-102+\frac{52\pi^2}{3}+\frac{4\pi^4}{45}+112\zeta(3)\right.\\
&\quad\left.-32\pi^2\zeta(3)+384\zeta(5)\right],\\
\delta^{(3)}_{\beta_0^3}E_3 &= E_3^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[32L_3^3+120L_3^2+\left(\frac{136}{3}+\frac{16\pi^2}{3}+192\zeta(3)\right)L_3-\frac{9514}{27}+\frac{427\pi^2}{9}+\frac{2\pi^4}{15}+140\zeta(3)\right.\\
&\quad\left.-72\pi^2\zeta(3)+864\zeta(5)\right],
\end{aligned} \tag{2}$$

where $L_n = \ln(n\mu/(C_F\alpha_s(\mu)m_q))$ and $\zeta(i)$ is Riemann's ζ function. The remaining contributions to $\delta E_n^{(3)}$ can be found in Ref. [8].

The perturbative expansion for the wave function can be written as follows

$$|\psi_n(0)|^2 \;=\; |\psi_n^C(0)|^2\left(1+\delta^{(1)}\psi_n+\delta^{(2)}\psi_n+\delta^{(3)}\psi_n+\ldots\right), \tag{3}$$

where $|\psi_n^C(0)|^2 = C_F^3\alpha_s^3 m_q^3/(8\pi n^3)$ is the leading order Coulomb value. Our result for the $\mathcal{O}(\beta_0^3\alpha_s^3)$ term reads

$$\begin{aligned}
\delta^{(3)}_{\beta_0^3}\psi_1 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[80L_1^3+\left(52-\frac{80\pi^2}{3}\right)L_1^2+\left(-40-6\pi^2+\frac{10\pi^4}{9}+200\zeta(3)\right)L_1\right.\\
&\quad\left.-20+\frac{22\pi^2}{3}-\frac{7\pi^4}{5}+\frac{4\pi^6}{105}+112\zeta(3)-12\pi^2\zeta(3)-16\zeta(3)^2-40\zeta(5)\right],\\
\delta^{(3)}_{\beta_0^3}\psi_2 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[80L_2^3+\left(332-\frac{160\pi^2}{3}\right)L_2^2+\left(308-\frac{266\pi^2}{3}+\frac{40\pi^4}{9}+400\zeta(3)\right)L_2\right.\\
&\quad\left.-361+\frac{73\pi^2}{3}-\frac{26\pi^4}{45}+\frac{32\pi^6}{105}+496\zeta(3)-48\pi^2\zeta(3)-128\zeta(3)^2-160\zeta(5)\right],\\
\delta^{(3)}_{\beta_0^3}\psi_3 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\left[80L_3^3+\left(612-80\pi^2\right)L_3^2+\left(\frac{2893}{3}-228\pi^2+10\pi^4+600\zeta(3)\right)L_3\right.\\
&\quad-\frac{100679}{54}+\frac{183\pi^2}{2}+\frac{52\pi^4}{15}+\frac{36\pi^6}{35}+1374\zeta(3)-108\pi^2\zeta(3)-432\zeta(3)^2
\end{aligned}$$

$$-360\zeta(5)\Bigg] \,. \tag{4}$$

In the next Section we discuss the numerical impact of the new terms to the system of two heavy quarks at threshold.

3. Phenomenological applications

3.1. Excited states of bottomonium

The mass of the $\Upsilon(nS)$ meson can be decomposed into perturbative and nonperturbative contributions

$$M_{\Upsilon(nS)} \;=\; 2m_b + E_n^{\rm p.t.} + \delta^{\rm n.p.}E_n \,. \tag{5}$$

As discussed in the previous Section, the perturbative contribution $E_n^{\rm p.t.}$ is know up to $\mathcal{O}(m_q\alpha_s^5)$. For $n = 1$ the phenomenological application of the result to the $\Upsilon(1S)$ meson mass has been discussed in Ref. [4] and a competitive extraction of the bottom quark mass has been obtained. It is thus tempting to investigate Eq. (5) also for excited states. In this context it is convenient to consider the ratio

$$\rho_n \;=\; \frac{E_n - E_1}{2m_b + E_1} \,, \tag{6}$$

which depends only logarithmically on the bottom quark mass and does not suffer from renormalon contributions.

Including successively higher orders one obtains for $\mu = \mu_s = 2.1$ GeV

$$\begin{aligned} 10^2 \times \rho_2^{\rm p.t.} &= 1.49\,(1 + 0.79_{\rm NLO} + 1.18_{\rm NNLO} + 1.21_{\rm N^3LO} + \ldots)\,, \\ 10^2 \times \rho_3^{\rm p.t.} &= 1.77\,(1 + 0.92_{\rm NLO} + 1.37_{\rm NNLO} + 1.55_{\rm N^3LO} + \ldots)\,. \end{aligned} \tag{7}$$

In Tab. I the sum of the individual orders is compared to the experimental result given by $\rho_n^{\rm exp} = (M_{\Upsilon(nS)} - M_{\Upsilon(1S)})/M_{\Upsilon(1S)}$. It is worth mentioning that although the convergence of the series is not good, the N^{3}LO perturbative result is in impressive agreement with the experimental values both for $n = 2$ and $n = 3$. We would like to emphasize the role of the perturbative corrections necessary to bring theory and experiment into agreement. From this observation one can conclude that the magnitude of the nonperturbative effects for the excited state, $\delta^{\rm n.p.}E_2$, is of the same size as $\delta^{\rm n.p.}E_1$. The latter was estimated to ≈ 60 MeV in Ref. [4]. Similar conclusion has been made in Ref. [20] in a somewhat different framework.

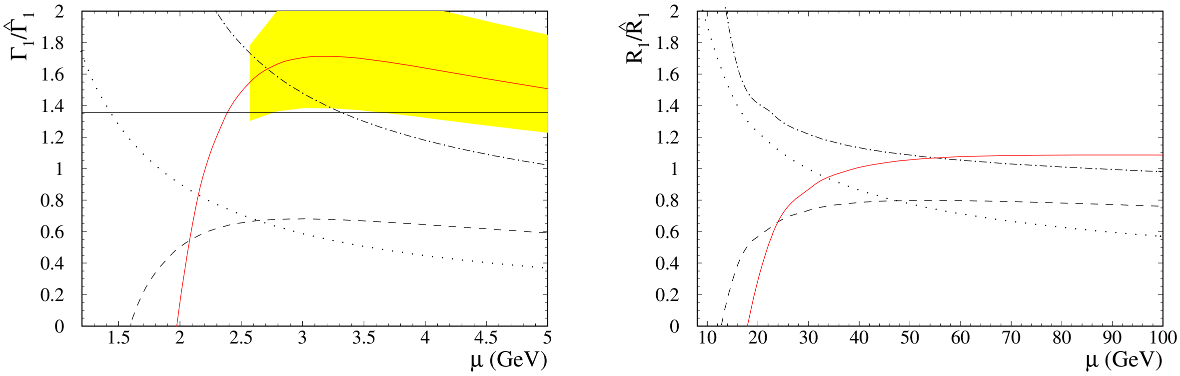
3.2. $\Upsilon(1S)$ leptonic width

It is tempting to use the new corrections to the wave function in order to predict the decay rate of the $\Upsilon(1S)$ meson into leptons. In the nonrelativistic effective theory the leading order approximation reads

$$\Gamma^{\rm LO}(\Upsilon(1S) \to l^+l^-) \;\equiv\; \Gamma_1^{\rm LO} \;=\; \frac{4\pi N_c Q_b^2 \alpha^2 |\psi_1^C(0)|^2}{3m_b^2} \,, \tag{8}$$

	$\Upsilon(2S)$	$\Upsilon(3S)$
$10^2 \times \rho_n^{\rm p.t.}$	$6.2^{+1.7}_{-1.2}$	$8.6^{+2.4}_{-1.8}$
$10^2 \times \rho_n^{\rm exp}$	5.95	9.46

Table I: Perturbative versus experimental results for the parameter ρ_n as defined in Eq. (6). The theoretical uncertainty corresponds to $\alpha_s(M_Z) = 0.118 \pm 0.003$.



(a) (b)

Figure 1: (a) Γ_1 normalized to $\hat{\Gamma}_1 \equiv \Gamma_1^{\rm LO}\big|_{\alpha_s\to\alpha_s(\mu_s)}$ as a function of μ at LO (dotted), NLO (dashed), NNLO (dotted-dashed) and N^{3}LO$'$ (full line). The horizontal line corresponds to the experimental value $\Gamma^{\rm exp}(\Upsilon(1S)\to e^+e^-) = 1.31$ keV. For the N^{3}LO$'$ result, the band reflects the errors due to $\alpha_s(M_Z) = 0.118\pm0.003$. (b) The analog plot for R_1 with $\hat{R}_1 \equiv R_1^{\rm LO}\big|_{\alpha_s\to\alpha_s(\mu_s)}$.

with $N_c = 3$ and $Q_b = -1/3$. Combining the known perturbative results up to $\mathcal{O}(\alpha_s^3\ln\alpha_s)$ (see Ref. [5]) with the $\mathcal{O}(\beta_0^3\alpha_s^3)$ contribution discussed in Section 2 we find

$$\Gamma_1 \;\approx\; \Gamma_1^{\rm LO}(1 - 0.445_{\rm NLO} + 1.75_{\rm NNLO} - 1.67_{\rm N^3LO'} + \ldots)\,, \tag{9}$$

where the prime indicates that the N^{3}LO corrections are not complete. Though the perturbative corrections are huge, the rapid growth of the perturbative coefficients stops at NNLO if we assume that the β_0^3 term sets the scale of the nonlogarithmic third-order contribution.

In Fig. 1(a), the width is plotted as a function of μ including the LO, NLO, NNLO and N^{3}LO$'$ approximations along with the experimental value. As one can see the available $\mathcal{O}(\alpha_s^3)$ terms stabilize the series and significantly reduce the scale dependence. At the scale $\mu' \approx 2.7$ GeV, which is close to the physically motivated scale μ_s, the N^{3}LO$'$ corrections vanish and at the scale $\mu'' \approx 3.1$ GeV the result becomes independent of μ; *i.e.*, the N^{3}LO$'$ curve shows a local maximum. In the whole range of μ between approximately 2 GeV and 5 GeV the result for the width agrees with the experimental value within the error bar due to the uncertainty of the strong coupling constant. This may signal that the missing perturbative corrections are rather moderate. Furthermore, this result constitutes a significant improvement as compared to the NLL approximation discussed in Ref. [21].

For a definite conclusion, however, one has to wait until the third-order corrections are completed. The potentially most important part to be computed is the ultrasoft contribution which includes $\alpha_s(\mu)$ normalized at relatively low ultrasoft scale $\mu_{us} \sim \alpha_s^2 m_q$. Currently only a partial result for this contribution exists [22].

3.3. Top quark threshold production

In contrast to the bottom system the nonperturbative effects in the case of the top quark are negligible. However, due to the relatively large top quark width, Γ_t, its effect has to be taken into account properly [23] since the Coulomb-like resonances below threshold are smeared out. Actually, the cross section only shows a small bump which is essentially the remnant of the ground state pole. The higher poles and continuum, however, affect the position of the resonance peak and move it to higher energy. The value of the normalized cross section $R = \sigma(e^+e^-\to t\bar{t})/\sigma(e^+e^-\to\mu^+\mu^-)$ at the resonance energy is dominated by the contribution from the *would-be* toponium ground state which in the leading approximation reads $R_1^{\rm LO} = 6\pi N_c Q_t^2 |\psi_1^C(0)|^2/\left(m_t^2\Gamma_t\right)$, where $Q_t = 2/3$. Numerically we find

$$R_1 \;\approx\; R_1^{\rm LO}(1 - 0.243_{\rm NLO} + 0.435_{\rm NNLO} - 0.268_{\rm N^3LO'} + \ldots)\,. \tag{10}$$

The new third-order corrections proportional to β_0^3 amount to approximately -7% of the LO approximation at the soft scale which is the same order of magnitude as the $\mathcal{O}(\alpha_s^3)$ linear logarithmic term. The available N^3LO terms improve the stability of the result with respect to the scale variation as can be seen in Fig. 1(b). The absence of a rapid growth of the coefficients along with the alternating-sign character of the series and the weak scale dependence suggest that the missing perturbative corrections are moderate and most likely are in the few-percent range. It is interesting to note that the perturbative contributions of different orders, which are relatively large when taken separately, cancel in the sum to give only a few percent variation of the leading order result.

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