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Leptonic decay of the Upsilon(1S) meson at third order in QCD

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We present the complete next-to-next-to-next-to-leading order short-distance and bound-state QCD correction to the leptonic decay rate $\Gamma(\Upsilon(1S) \to \ell^+\ell^-)$ of the lowest-lying spin-1 bottomonium state. The perturbative QCD prediction is compared to the measurement $\Gamma(\Upsilon(1S) \to e^+e^-) = 1.340(18)$ keV.

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Bound states of a heavy quark and antiquark provide an ideal laboratory to study non-relativistic quantum chromodynamics (NRQCD). The bound-state dynamics is characterized by three scales, the mass of the heavy quark (hard scale), m, its typical momentum (soft scale), mv, and energy (ultrasoft scale), mv^2. Here $v \sim \alpha_s(mv)$ is the velocity of the quark in the bound state and α_s the strong coupling. The theoretical description of heavy-quark bound states uses the fact that the different scales are well-separated since the velocity is small. This allows to construct a series of effective theories by integrating out the larger scales. Starting from QCD, the first step is to integrate out the hard modes to obtain NRQCD [1–3]. The second step is to integrate out potential and soft gluons and soft light quarks, leading to potential NRQCD (PNRQCD) [4]. PNRQCD contains only potential heavy quarks, whose energy and momentum are of order mv^2 and mv, respectively, and ultrasoft gluons and light quarks.

A "classical" application of NRQCD is the prediction of the decay rate of heavy-quark bound states into leptons. The simplest such system is the $\Upsilon(1S)$ meson, the lowest-lying spin-triplet bound state of a bottom quark and antiquark. To next-to-next-to-next-to-leading order accuracy (N^{3}LO) the decay rate can be computed with the help of the formula [5]

$$\Gamma(\Upsilon(1S) \to \ell^+\ell^-) = \frac{4\pi\alpha^2}{9m_b^2}\,|\psi_1(0)|^2\, c_v \left[c_v - \frac{E_1}{m_b}\left(c_v + \frac{d_v}{3}\right) + \ldots\right], \quad (1)$$

with α being the fine structure constant and m_b the bottom-quark pole mass. c_v and d_v are matching constants of leading and sub-leading $b\bar{b}$ currents in NRQCD, and $\psi_1(0)$ is the wave function of the $(b\bar{b})$ system at the origin, which at leading order is given by

$$\left|\psi_1^{\rm LO}(0)\right|^2 = \frac{8m_b^3\alpha_s^3}{27\pi}\,. \quad (2)$$

The mass of the $\Upsilon(1S)$ is $M_{\Upsilon(1S)} = 2m_b + E_1$, and the perturbative part of the binding energy E_1 is given at leading order by $E_1^{p,\rm LO} = -(4m_b\alpha_s^2)/9$.

In the following we assume that the bound-state dynamics of the $\Upsilon(1S)$ state is governed by weak coupling, which formally requires that the ultrasoft scale $m_b v^2$ is large compared to the strong interaction scale Λ. It is generally believed that this is a reasonable assumption for the lowest-lying $1S$ state, but not for the higher states, which, though more non-relativistic, are too large to be considered as bound states dominated by the colour-Coulomb interaction. Even for the $1S$ state the assumption $m_b v^2 \gg \Lambda$ is questionable. In fact, the leptonic decay that we consider in this Letter should be considered as one of the crucial tests of perturbative QCD bound-state dynamics, when all three scales (hard, soft, ultrasoft) are relevant to the problem. The more recent analyses of the leptonic $\Upsilon(1S)$ decay are based on next-to-leading order QCD together with non-perturbative condensate corrections [6], or second-order QCD without non-perturbative corrections [7], and both fail to describe the measured decay width accurately. The problem arises from large uncertainties in the perturbative and non-perturbative corrections. We address both issues in this Letter.

Recently the last missing ingredients for a complete N^{3}LO evaluation of $\Gamma(\Upsilon(1S) \to \ell^+\ell^-)$ have been computed, which allow us to reconsider the problem with unprecedented accuracy: The gluonic three-loop contributions to c_v have been evaluated in Ref. [8], and third-order corrections to the wave function at the origin induced by single- and double-potential insertions and ultrasoft gluon exchange are computed in Ref. [5, 9–11]. Furthermore, the still missing two-loop $\mathcal{O}(\epsilon)$ term of the $d = 4 - 2\epsilon$ dimensional matching coefficient of the $1/(m_b r^2)$ PNRQCD potential is given in the Appendix.

Thus, we are now in the position to compute the decay rate of the $\Upsilon(1S)$ meson into a lepton pair to third order in perturbation theory. The following results apply to the cases $\ell = e, \mu$, where the lepton mass can be neglected. Expanding out all factors of Eq. (1) in $\alpha_s \equiv \alpha_s(\mu)$, where μ denotes the renormalization scale in the $\overline{\mathrm{MS}}$ scheme, we obtain

$$\begin{aligned}
&\Gamma(\Upsilon(1S) \to \ell^+\ell^-)|_{\mathrm{pole}} \\
&= \frac{2^5\alpha^2\alpha_s^3 m_b}{3^5}\Big[1 + \alpha_s\left(-2.003 + 3.979\,L\right) \\
&\quad + \alpha_s^2\left(9.05 - 7.44\,\ln\alpha_s - 13.95\,L + 10.55\,L^2\right) \\
&\quad + \alpha_s^3\big(-0.91 + 4.78_{a_3} + 22.07_{b_{2\epsilon}} + 30.22_{c_f} \\
&\qquad - 134.8(1)_{c_g} - 14.33\,\ln\alpha_s - 17.36\,\ln^2\alpha_s \\
&\qquad + (62.08 - 49.32\,\ln\alpha_s)\,L - 55.08\,L^2 \\
&\qquad + 23.33\,L^3\big) + \mathcal{O}(\alpha_s^4)\Big] \qquad (3) \\
&= \frac{2^5\alpha^2\alpha_s^3 m_b}{3^5}\left[1 + 1.166\alpha_s + 15.2\alpha_s^2 + (66.5 + 4.8_{a_3}\right. \\
&\quad \left. + 22.1_{b_{2\epsilon}} + 30.2_{c_f} - 134.8(1)_{c_g})\,\alpha_s^3 + \mathcal{O}(\alpha_s^4)\right] \\
&= \frac{2^5\alpha^2\alpha_s^3 m_b}{3^5}\left[1 + 0.28 + 0.88 - 0.16\right] \\
&= [1.04 \pm 0.04(\alpha_s)^{+0.02}_{-0.15}(\mu)]\ \mathrm{keV}\,, \qquad (4)
\end{aligned}$$

where $L = \ln(\mu/(m_b C_F \alpha_s))$ with $C_F = 4/3$. The subscripts indicate the contribution from the (scale independent) coefficients of the three-loop static potential (a_3), the $\mathcal{O}(\epsilon)$ term of the $1/(m_b r^2)$ potential ($b_2\epsilon$) and the fermionic and bosonic contribution of the three-loop matching coefficient (c_f and c_g). The uncertainty due to the limited precision of the latter is given in parentheses. The contribution from the $\mathcal{O}(\epsilon)$ terms of the $1/(m_b^2 r^3)$ potentials is not made explicit.

For the numerical evaluation after Eq. (3) we use $\alpha(2m_b) = 1/132.3$ [12], $\alpha_s(M_Z) = 0.1184(10)$ and the renormalization scale $\mu = 3.5$ GeV. We use the program `RunDec` [13] to evolve the coupling in the four-loop approximation such that $\alpha_s(3.5\,\mathrm{GeV}) = 0.2411$ and to compute the pole mass $m_b = 4.911$ GeV in the 3-loop approximation from the $\overline{\mathrm{MS}}$ value $\bar{m}_b(\bar{m}_b) = 4.163(16)$ GeV given in Ref. [14]. The scale uncertainty in Eq. (4) is computed from the maximum and minimum value of the width within the range $\mu \in [3, 10]\,\mathrm{GeV}$ (see discussion below). Note that the uncertainty induced by the bottom-quark mass is below 1 per mille and can thus be neglected. However, this does not take into account the uncertainty due to the perturbative instability of the pole mass.

We can avoid the computation of the pole mass by going to the potential-subtracted (PS) mass scheme [15]. In computing the PS mass from the $\overline{\mathrm{MS}}$ mass $\bar{m}_b(\bar{m}_b) = 4.163$ GeV, we combine (for $n = 1, 2, 3$) the n-loop correction to the $\overline{\mathrm{MS}}$-pole-mass relation with the $(n-1)$-loop correction to the Coulomb potential in the pole-PS-mass relation and find $m_b^{\mathrm{PS}} \equiv m_b^{\mathrm{PS}}(\mu_f = 2\,\mathrm{GeV}) = 4.484$ GeV. We then eliminate m_b in Eq. (3) by replacing $m_b = m_b^{\mathrm{PS}} + \delta m$ and expand systematically in α_s to obtain

$$\begin{aligned}
&\Gamma(\Upsilon(1S) \to \ell^+\ell^-)|_{\mathrm{PS}} \\
&= \Gamma(\Upsilon(1S) \to \ell^+\ell^-)|_{\mathrm{pole}, m_b \to m_b^{\mathrm{PS}}} \\
&\quad + \frac{2^5\alpha^2\alpha_s^3 m_b^{\mathrm{PS}}}{3^5}\,x_f\Big[0.42\alpha_s^2 + \alpha_s^3\big(-1.78 + 0.28\,L_f \\
&\qquad + 1.69\,L\big) + \mathcal{O}(\alpha_s^4)\Big] \qquad (5) \\
&= \frac{2^5\alpha^2\alpha_s^3 m_b^{\mathrm{PS}}}{3^5}\left[1 + 1.528\alpha_s + 16.3\alpha_s^2 + (74.7 + 4.8_{a_3}\right. \\
&\quad \left. + 22.1_{b_{2\epsilon}} + 30.2_{c_f} - 134.8(1)_{c_g})\,\alpha_s^3 + \mathcal{O}(\alpha_s^4)\right] \\
&= \frac{2^5\alpha^2\alpha_s^3 m_b^{\mathrm{PS}}}{3^5}\left[1 + 0.37 + 0.95 - 0.04\right] \\
&= [1.08 \pm 0.05(\alpha_s)^{+0.01}_{-0.20}(\mu)]\ \mathrm{keV}\,, \qquad (6)
\end{aligned}$$

with $x_f = \mu_f/(m_b^{\mathrm{PS}}\,\alpha_s)$ and $L_f = \ln(\mu^2/\mu_f^2)$. The pattern of the series is essentially the same in both schemes. The NNLO corrections are very large [7], but we find only moderate corrections at N^{3}LO. Together with the improved scale dependence at third order discussed below, this may be an indication that perturbative corrections beyond the third order are small.

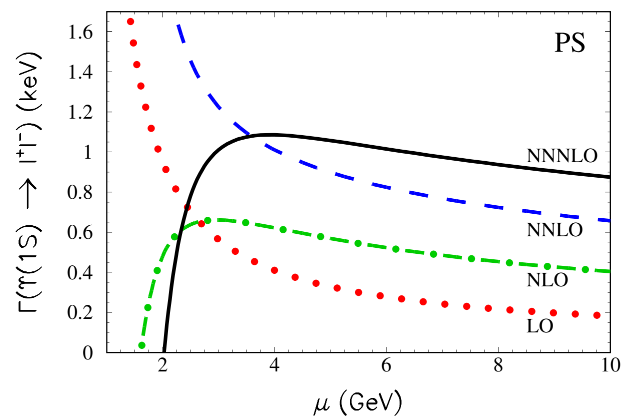

FIG. 1. The decay rate in the PS scheme as a function of the renormalization scale μ. Dotted (red), dash-dotted (green), short-dashed (blue) and solid (black) lines correspond to LO, NLO, NNLO and N^{3}LO prediction.

In Fig. 1 we show the decay rate $\Gamma(\Upsilon(1S) \to \ell^+\ell^-)$ in the PS scheme as a function of the renormalization scale including successively higher orders. Very similar results are obtained for the pole scheme. For small scales no convergence is observed and for values close to the soft scale $\mu_s = m_b\alpha_s(\mu_s)C_F \approx 2.0$ GeV there are big differences between subsequent perturbative orders. It is interesting to note that for $\mu \gtrsim 3$ GeV the N^{3}LO prediction becomes quite flat and furthermore only shows a small deviation from the NNLO curve. We take this as evidence that perturbative computations of Coulomb bound states in QCD are better behaved when the scale is taken somewhat larger than the naive estimate of the soft scale, as

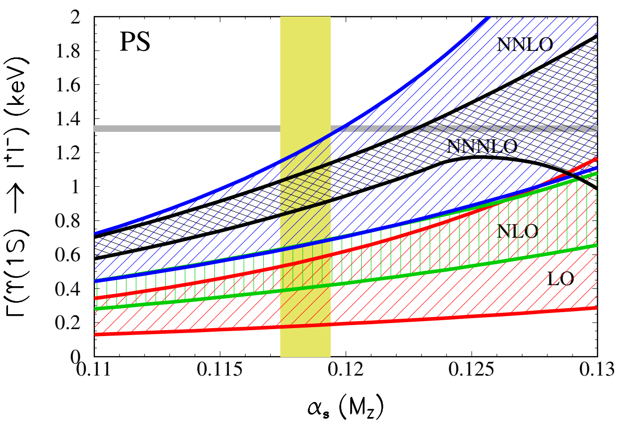

FIG. 2. The decay rate as a function of $\alpha_s(M_Z)$ at LO (red, bottom), NLO (green, middle), NNLO (blue, top), and N^{3}LO (black, inner top band). The bands denote the variation of μ between 3 GeV and 10 GeV. The horizontal bar denotes the experimental value, while the vertical bar denotes the world average of the strong coupling constant, $\alpha_s(M_Z) = 0.1184(10)$.

already observed in Ref. [16], and vary μ between 3 GeV and 10 GeV to compute the scale uncertainty.

Compared to the experimental value $\Gamma(\Upsilon(1S) \to e^+e^-)|_{\rm exp} = 1.340(18)$ keV [17], the third-order perturbative result is about 30% too low. The discrepancy remains substantial even when including the theoretical uncertainty. Note, however, that the decay rate depends on the value of α_s to a high power. In Fig. 2 we therefore show the decay rate and its scale dependence as a function of $\alpha_s(M_Z)$ at LO, NLO, NNLO, and N^{3}LO in the PS scheme. The plot shows good convergence of the perturbative series up to $\alpha_s(M_Z) \approx 0.122$, with the N^{3}LO band completely inside the NNLO one. However, the third-order result is always below the experimental value up to this point.

Since the perturbative contributions seems to be well under control at third order, a possible explanation for the difference between the experimental and the perturbative value is a sizable non-perturbative contribution. This is not implausible, since the scale of ultrasoft gluons is close to the strong-interaction scale for the $\Upsilon(1S)$ meson. The contribution to the wave function at the origin due to the gluon condensate has been evaluated in Refs. [6, 18]. It takes the form

$$\delta_{\rm np}|\psi_1(0)|^2 = |\psi_1^{\rm LO}(0)|^2 \times 17.54\pi^2 K\,, \tag{7}$$

where

$$K = \frac{\langle \frac{\alpha_s}{\pi} G^2 \rangle}{m_b^4 (\alpha_s C_F)^6} \tag{8}$$

is the dimensionless number that controls the relative size of the gluon condensate contribution. Using $\langle \frac{\alpha_s}{\pi} G^2 \rangle = 0.012$ GeV^4 [19] and $\alpha_s(3.5\,\text{GeV})$, its contribution to the decay rate evaluates to $\delta_{\rm np}\Gamma_{\ell\ell}(\Upsilon(1S)) = 1.67$ keV in the pole mass scheme and 2.20 keV in the PS mass scheme, far in excess of the missing 0.26 keV. There is a large uncertainty in these estimates, since the value of the gluon condensate is very uncertain and the scale of α_s in the denominator is undetermined. For example, if we adopt the strategy of Ref. [6] and replace α_s in the denominator of Eq. (8) by a coupling $\tilde{\alpha}_s$ related to the coefficient of the Coulomb potential at the scale $\mu = 1$ GeV, the above numbers change to 0.06 keV (pole scheme) and 0.08 keV (PS scheme), respectively. Moreover, depending on the choice for the strong coupling in Eq. (8), one either concludes from the size of the dimension-6 condensate contribution, also computed in Ref. [6], that the condensate expansion is not convergent, or, to the contrary, well behaved. Hence, no reliable estimate of the leptonic decay width can be obtained by this procedure.

Additional insight on $\delta_{\rm np}|\psi_1(0)|^2$ can be obtained from the mass of the $\Upsilon(1S)$ state, which we can write as

$$M_{\Upsilon(1S)} = 2m_b + E_1^{\rm p} + \frac{624\pi^2}{425}\, m_b (\alpha_s C_F)^2 K\,, \tag{9}$$

where $E_1^{\rm p}$ is the perturbative contribution to the bound-state energy, which is also known to the third order in QCD [16, 20, 21], and K is the gluon condensate correction from Refs. [6, 18, 22]. For the following analysis, it is mandatory to work with the PS scheme to achieve a reliable perturbative expansion of E_1^p (cf. Ref. [16], Eq. (38)). A direct determination of $m_b^{\rm PS}$ from the $\Upsilon(1S)$ mass at third order, but excluding the non-perturbative contribution, gives $m_b^{\rm PS} = 4.57$ GeV [16] (the central scale $\mu \approx 2$ GeV is used in this reference), which is larger than the value 4.48 GeV obtained above from the most accurate determinations of the $\overline{\rm MS}$ bottom-quark mass. This suggests that there is a non-negligible non-perturbative contribution $\delta M^{\rm np}_{\Upsilon(1S)}$ to the $\Upsilon(1S)$ mass. Repeating the analysis of Ref. [16] with our parameters, we find

$$\begin{aligned} \delta M^{\rm np}_{\Upsilon(1S)} &\equiv M_{\Upsilon(1S)} - (2m_b^{\rm PS} + E_1^{\rm p,PS}) \\ &\approx [125 \pm 16(\alpha_s) \pm 34(m_b)^{+10}_{-25}(\mu)]\,\text{MeV}\,, \end{aligned} \tag{10}$$

where $E_1^{\rm p,PS} = 2m_b - 2m_b^{\rm PS} + E_1^p$. This estimate is considerably larger than the value $\delta M^{\rm np}_{\Upsilon(1S)} \approx 15$ MeV given in Ref. [6] based on the condensate expansion, and relies only on the accurate input value for the bottom $\overline{\rm MS}$ mass and the convergence of the perturbative expansion of the binding energy in the PS scheme [16].

Eq. (10) neglects the mass of the charm quark. The effect of a finite mass $m_c = 1.4$ GeV is easily computed at $\mathcal{O}(\alpha_s^2)$ and reduces $\delta M^{\rm np}_{\Upsilon(1S)}$ by 12 MeV for given $\overline{\rm MS}$ bottom-quark mass. Including an estimate of the next order from Ref. [23], we therefore subtract (20 ± 10) MeV from Eq. (10). Comparing Eq. (9) to Eq. (7), we find the relation

$$\begin{aligned} \delta_{\rm np}\Gamma_{\ell\ell}(\Upsilon(1S)) &= \frac{4\alpha^2\alpha_s}{9}\,\frac{17.54\times 425}{3744}\,\delta M^{\rm np}_{\Upsilon(1S)} \\ &\approx [1.28^{+0.17}_{-0.18}(\alpha_s) \pm 0.42(m_b)^{+0.20}_{-0.57}(\mu) \pm 0.12(m_c)]\,\text{keV}\,. \end{aligned} \tag{11}$$

The numerical result is closer to the larger values obtained in our previous estimates. It must, however, be taken with a grain of salt, since for such large values the condensate expansion is not convergent. The different sub-leading dimension-6 corrections to $\delta_{\rm np}\Gamma_{\ell\ell}(\Upsilon(1S))$ and $\delta M^{\rm np}_{\Upsilon(1S)}$ then invalidate the simple relation (11) and once again preclude a reliable estimate of the non-perturbative part of the leptonic decay width. We should emphasize that this conclusion depends strongly on the state-of-the-art value $\bar{m}_b(\bar{m}_b) = 4.163(16)$ GeV of the $\overline{\rm MS}$ mass [14]. If the mass were only 40 MeV larger, we would find $\delta_{\rm np}\Gamma_{\ell\ell}(\Upsilon(1S)) \approx 0.3\,$keV from Eq. (11) and simultaneously conclude that the condensate expansion is well behaved.

In summary, we have computed the third-order correction to the decay rate $\Gamma(\Upsilon(1S) \to l^+l^-)$. This is the first third-order QCD bound-state calculation, where both short- and long-distance effects are important. Both in the pole and potential subtracted scheme the N^{3}LO corrections are negative and amount to about -16% and -4%, respectively. The perturbative uncertainty that constituted the main limitation of previous analyses is thus mostly removed. We find that the leptonic decay width is mostly perturbative; the perturbative contribution amounts to roughly 70% of the measured value. The new third-order contribution is crucial to ascertain this conclusion. We further considered several estimates of non-perturbative effects based on the condensate expansion, including a relation to the mass of the $\Upsilon(1S)$ state. Unfortunately, the situation is ambiguous and no clear conclusion on the size of non-perturbative effects could be drawn. Whether a full quantitative, theoretical understanding of the leptonic decay width can be achieved therefore remains an open question. We note, however, that this conclusion relies on the precise value of the bottom $\overline{\rm MS}$ quark mass.

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APPENDIX: TWO-LOOP $\mathcal{O}(\epsilon)$ TERM OF $1/(m_b r^2)$ POTENTIAL

In this Appendix we present the result for the two-loop $\mathcal{O}(\epsilon)$ term of the matching coefficient of the $1/(m_b r^2)$ potential. This is most easily achieved by replacing the quantity b_2 in Eq. (6) of Ref. [24] by $b_2 + \epsilon b_2^\epsilon$. Then b_2^ϵ reads

$$\begin{aligned} b_2^\epsilon = {} & C_F C_A \left(-\frac{631}{108} - \frac{15\pi^2}{16} + \frac{65\ln 2}{9} - \frac{8\ln^2 2}{3} \right) \\ & + C_A^2 \left(-\frac{1451}{216} - \frac{161\pi^2}{72} - \frac{101\ln 2}{18} - \frac{4\ln^2 2}{3} \right) \\ & + C_A T n_l \left(\frac{115}{54} + \frac{5\pi^2}{18} + \frac{49\ln 2}{18} \right) \\ & + C_F T n_l \left(\frac{17}{27} - \frac{11\pi^2}{36} - \frac{4\ln 2}{9} \right) . \end{aligned} \tag{12}$$

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