Bottom and Charm Quark Mass Determination from Quarkonium at N^{3}LO

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The non-perturbative nature of QCD at hadronic scales implied the development of phenomeno-logical approaches such as quark models or, more recently, computer-based calculations using Lattice QCD. However, the unique properties of heavy quarkonium systems allow an entire calculation in terms of non-relativistic perturbative QCD. In this work, the bottomonium spectrum, up to $n = 3$, and the ground state charmonium states, are analyzed in the framework of Non-Relativistic Quantum Chromodynamics at N^{3}LO. For bottomonium, finite charm quark mass effects in the QCD potential and the $\overline{\text{MS}}$-pole mass relation are incorporated to the highest known order, $\mathcal{O}(\varepsilon^3)$ in the Υ-scheme counting. The bottom quark pole mass is expressed in terms of the MSR mass, a low-scale short-distance mass which cancels the $u = 1/2$ renormalon of the static potential. We study the $n_\ell = 3$ and $n_\ell = 4$ schemes, finding a negligible difference between the two if finite m_c effects are smoothly incorporated in the MSR mass definition. We find that bottomonium $n = 3$ states are not well behaved within perturbative NRQCD. Hence, fitting to the $n = 1, 2$ $b\bar{b}$ states we obtain $\overline{m}_b(\overline{m}_b) = 4.216 \pm 0.039$ GeV. Similarly, from the lowest lying charmonium states we find $\overline{m}_c(\overline{m}_c) = 1.273 \pm 0.054$ GeV.

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1. Introduction

Heavy quarkonium systems are unique, as their dynamics allow a full calculation using non-relativistic QCD (NRQCD) with perturbative methods. Within NRQCD the calculation of the energy levels of heavy quarkonium relies on the accurate description of the static QCD potential $V_{QCD}(r)$. Most recent calculations computed the energy levels of the lower-lying bottomonium states up to $\mathcal{O}(\alpha_s^5 m)$ and $\mathcal{O}(\alpha_s^5 m \log \alpha_s)$ using pNRQCD [1], which describes the interactions of a non-relativistic system with ultrasoft gluons organizing the perturbative expansions in α_s and the velocity of heavy quarks systematically. A closed expression for arbitrary quantum numbers can be found in [2].

The convergence of the perturbative expansion depends, though, on the short-distance mass scheme employed to ensure the $\mathcal{O}(\Lambda_{QCD})$ renormalon cancellation. The authors of Ref. [3] employed the well-known $\overline{MS}$ scheme, commonly used for physical situations in which the relevant scale is of the order or larger than the heavy quark mass. For heavy quarkonium the typical scale is much smaller, therefore the results can be substantially improved by switching to a low-scale short-distance scheme.

In this work we study the predictions for the energy levels of heavy quarkonium at N^3LO using the MSR scheme [4], and determine the bottom quark mass, including finite charm quark mass effects, using states with $n \leq 3$ and the charm quark mass from the low-lying charmonium spectrum. A careful study of scale variation is performed, using the idea that the argument of perturbative logarithms should roughly vary between $1/2$ and 2, while keeping at all times the renormalization scale above $1\,\text{GeV}$ such that perturbation theory is still valid. A more detailed description of this work has been recently presented in Ref. [5]. The reader is kindly referred to the latter work for further details.

2. Computation of $Q\overline{Q}$ Bound States

The energy of a non-relativistic $Q\overline{Q}$ bound state with arbitrary quantum numbers and with n_ℓ massless active flavors reads, in the pole scheme reads [6, 7, 2]:

$$E_X(\mu, n_\ell) = 2m_Q^{\text{pole}} \left[1 - \frac{C_F^2 \, \alpha_s^{(n_\ell)}(\mu)^2}{8n^2} \sum_{i=0}^{\infty} \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i \varepsilon^{i+1} P_i(L_{n_\ell}) \right], \quad (2.1)$$

with

$$L_{n_\ell} = \log \left(\frac{n\mu}{C_F \alpha_s^{(n_\ell)}(\mu) m_Q^{\text{pole}}} \right) + H_{n+\ell}, \qquad P_i(L_{n_\ell}) = \sum_{j=0}^{i} c_{i,j} L_{n_\ell}^j, \quad (2.2)$$

where H_n is the harmonic number and ε is a bookkeeping parameter used to organize the various orders in the Υ-expansion scheme. Imposing μ independence of the energy levels, the $c_{i,j}$ coefficients can be recursively calculated from $c_{i,0}$, which have been calculated up to $i = 3$ in Refs. [8, 9].

A precise determination of the heavy quark masses directly from Eq. (2.1) is inadequate, as such equation inherits the $u = 1/2$ renormalon of the static potential. Thus, the pole mass must be expressed in terms of a short-distance mass. Furthermore, a low-scale short-distance mass is advisable to avoid large logarithms of the ratio of the non-relativistic scale and the quark mass. In this work, two equivalent versions of the MSR mass [10, 4] will be used.

The MSR scheme was built as a natural extension of the $\overline{\text{MS}}$ mass for renormalization scales below the heavy quark mass. Its definition is derived directly from the $\overline{\text{MS}}$-pole mass relation and, in contrast with the $\overline{\text{MS}}$ mass, which has only logarithmic dependence on the scale μ, MSR mass has logarithmic and linear dependence on an infrared scale R :

$$\delta m_Q^{\text{MSR}} \equiv m_Q^{\text{pole}} - m_Q^{\text{MSR}}(R) = R \sum_{n=1}^{\infty} a_n(n_\ell) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^n . \tag{2.3}$$

The a_n are derived from the $\overline{\text{MS}}$ pole mass relation, and are different for the *practical* and *natural* versions of the MSR mass, which are two alternative but equivalent ways to change from a scheme with $(n_\ell + 1)$ dynamical flavors to another with only n_ℓ. On the one hand, the *practical* MSR *mass* (MSRp) uses the threshold matching relation of the strong coupling to rewrite $\alpha_s^{(n_\ell+1)}(\overline{m})$ in terms of $\alpha_s^{(n_\ell)}(\overline{m})$ and, on the other hand, the *natural* MSR *mass* (MSRn) directly integrates out the heavy quark Q from the $\overline{\text{MS}}$ to pole relation setting all diagrams with heavy quark loops to zero.

The R dependence of the MSR mass is described by :

$$- \frac{\mathrm{d}}{\mathrm{d}R} m_Q^{\text{MSR}}(R) = \gamma^R[\alpha_s^{(n_\ell)}(R)] = \sum_{n=0}^{\infty} \gamma_n^R \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^{n+1} , \tag{2.4}$$

where $\gamma_n^R = a_{n+1} - 2\sum_{j=0}^{n-1}(n-j)\beta_j a_{n-j}$ are the R-anomalous dimension coefficients [4].

Effects from the finite charm quark mass contribute to the relation of the pole mass to the MSR mass and to Eq. (2.1). Corrections to the binding energy result in an energy-shift to the heavy quarkonium mass and have been calculated up to $\mathcal{O}(\varepsilon^3)$ [11, 12, 13]. In the pole mass scheme they can be written as :

$$E_X(\mu, n_\ell, m_Q^{\text{pole}}, m_q^{\text{pole}}) = E_X(\mu, n_\ell, m_Q^{\text{pole}}) + \varepsilon^2 \delta E_X^{(1)} + \varepsilon^3 \delta E_X^{(2)} . \tag{2.5}$$

The exact $\delta E_X^{(2)}$ term has only been computed for the $\ell = 0$ bottomonium states [12, 13]. For the rest of states we follow the approach used in Ref. [8], where the authors employ the $m_c \to \infty$ limit, which we complete by requiring that the correction in the n_ℓ scheme vanishes for $m_c \to 0$.

The corrections from the finite charm quark mass to the MSR-pole mass relation start at $\mathcal{O}(\alpha_s^2)$:

$$\delta m_Q^{\text{MSR}}(R, \overline{m}_c) = \delta m_Q^{\text{MSR}}(R) + R \sum_{k=2} \Delta_{\overline{m}_c}^{(k)}(\xi) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^k , \tag{2.6}$$

where $\xi = \overline{m}_c/R$ and δm_Q^{MSR} is given in Eq. (2.3). The ε^2 correction term has been calculated exactly in Ref. [14]. The ε^3 correction was analytically calculated in Ref. [15], but due to its complexity we have used a numerical approximation using a Padè parametrization, which is accurate up to 8 significant digits in the range $0 \le \xi \le 1$, enough for our purposes [5].

The aforementioned finite charm mass corrections also modify the R-anomalous dimension :

$$- \frac{\mathrm{d}}{\mathrm{d}R} m_Q^{\text{MSR}}(R) = \gamma^R[\alpha_s^{(n_\ell)}(R)] + \sum_n \delta\gamma_n^R(\xi) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^{n+1} , \tag{2.7}$$

with $\delta\gamma_n^R(\xi) = \Delta_n(\xi) - \xi \frac{d\Delta_n(\xi)}{d\xi} - 2\sum_{j=0}^{n-2}(n-j)\beta_j\Delta_{n-j}(\xi)$.

The $\mathcal{O}(\alpha_s^4)$ finite charm quark mass corrections are unknown so in our calculations we will cut the propagation of $\Delta_{\overline{m}_c}^{(2,3)}(\xi)$ terms to the $\mathcal{O}(\varepsilon^4)$ order, in order to avoid possible cancellations among crossed terms.

Up to now we have explicitly account for the charm mass corrections in the n_ℓ scheme. Alternatively, one can integrate out the charm quark, as it is sufficiently large compared to typical NRQCD scales to assume it is near the decoupling limit ($\overline{m}_c \to \infty$). Therefore we will study, together with the n_ℓ scheme with charm quark mass corrections, a scheme with $(n_\ell - 1)$ dynamical flavors.

3. Results

Our aim is to extract the $\overline{\text{MS}}$ bottom and charm masses from the perturbative expression for the mass of heavy quarkonium states, contained in Eq. (2.1) in the MSR mass scheme, fitting it against experimental values from the PDG. For a given dataset, $\overline{m}_Q$ is obtained from the minimum of the following χ^2 function, which depends on a set of pairs of renormalization scales $\{\mu_n, R_n\}$, where the index n runs over each principal quantum number in the dataset:

$$\chi^2(\{\mu_n, R_n\}) = \sum_i \left(\frac{M_i^{\text{exp}} - M_i^{\text{pert}}(\mu_i, R_i, \overline{m}_Q)}{\sigma_i^{\text{exp}}}\right)^2. \tag{3.1}$$

The previous sum extends to the individual heavy quarkonium states in the dataset and M_i^{exp} and σ_i^{exp} are the experimental masses and errors extracted from the PDG [16]. Such fit would give us a best-fit $\overline{\text{MS}}$ mass value as a function of the $\{\mu_n, R_n\}$ pair. This approach is taken because the theoretical uncertainties are highly correlated among various states and the so-called d'Agostini bias [17] emerges, which states that the global best-fit value is considerably lower than individual determinations from each state in the set. An alternative way is to perform a weighted average of the best-fit results. Both methods are in quite good agreement, though this last option leads to slightly larger perturbative uncertainties.

The renormalization scales μ and R are varied independently, within reasonable ranges, to estimate the the perturbative uncertainties. Such ranges depend on the convergence behavior for each heavy quarkonium state. Our procedure is to select ranges where the argument of the perturbative logarithms are roughly unity. This implies that, for $n = 1$ and $n = 3$ states, the renormalization scales should be varied between $(\mu_1, R_1) \in [1.5, 4]\,\text{GeV}$, whereas for states with $n = 2$ the range $(\mu_2, R_2) \in [1, 4]\,\text{GeV}$ is preferred. For charmonium we use the range $1.2\,\text{GeV} \geq \mu_{\text{charm}} \geq 4\,\text{GeV}$, which gives a pattern very similar to the $n = 1$ bottomonium states. It is worth noticing that the μ_n and R_n scales have to be varied together to account for theoretical correlations.

From the χ^2 minimization we obtain the central value of $\overline{m}_Q$, calculated as the average of all the best-fits in the (μ, R) grid, and the uncertainty coming from the experimental error of the heavy quarkonium masses, denoted as Δ^{exp}, also taken as the average in the grid.

The largest source of error is the one associated to the variation of the scales, that is, Δ^{pert}. Its value is calculated as the difference of the maximum and minimum best-fit values in the grid. Finally, there are additional errors originating from the uncertainty on the strong coupling Δ^{α_s} and, for the bottom (charm) mass fits, the charm (bottom) mass $\Delta^{\overline{m}_c}$ ($\Delta^{\overline{m}_b}$).
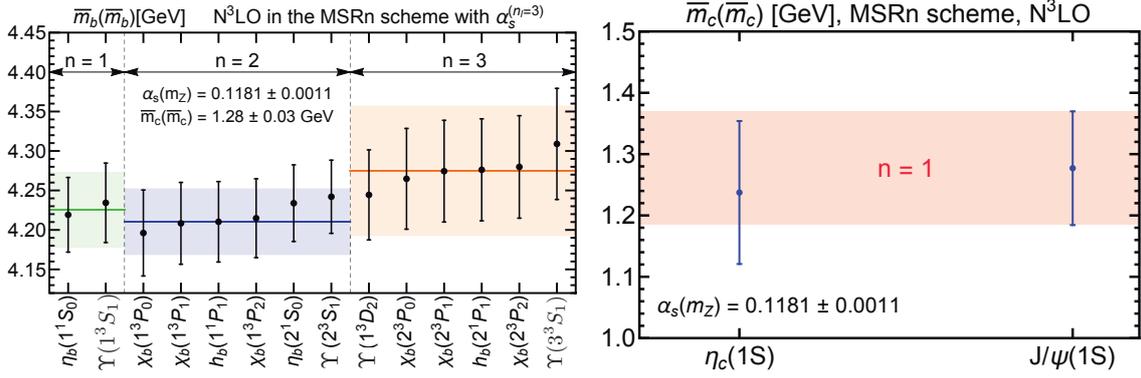
Figure 1: Left panel : Bottom quark mass determinations from individual fits to bottomonium states with principal quantum number $n \leq 3$ (black dots with error bars) and global fits to $n = 1$ (green band), $n = 2$ (blue band), and $n = 3$ states (orange band). All computations at N^3LO in the MSRn scheme with $n_\ell = 3$ active flavors. Right panel : Same for charm quark mass. Both panels : only perturbative uncertainties shown.

We have carried out fits for 14 individual bottomonium states (all states with $n \leq 3$) and global fits for sets with $n = 1$ states, $n = 2$ states, $n = 3$ states, and different combinations such as all states with $n \leq 2$ and $n \leq 3$. Our results are shown in Fig. 3 for the MSRn scheme with $n_\ell = 3$.

The expansion with $n_\ell = 3$ flavors is favored over $n_\ell = 4$, as suggested by Ref. [18]. We consider the set with $n \leq 2$ states as our default, as such states can be accurately described within perturbation theory. We take the MSRn scheme (which is theoretically cleaner) as our default, finding our final result for the bottom mass :

$$\overline{m}_b(\overline{m}_b) = 4.216 \pm 0.009_{\text{exp}} \pm 0.034_{\text{pert}} \pm 0.017_{\alpha_s} \pm 0.0008_{\overline{m}_c} \, \text{GeV} = 4.216 \pm 0.039 \, \text{GeV}. \quad (3.2)$$

The perturbative uncertainty clearly dominates over the rest, followed by the error from the strong coupling. The error due to the uncertainty on the charm mass is negligible, as the experimental one.

Equivalently, the charm mass can be obtained from $c\bar{c}$ bound state calculations via Eq. (2.1). We will restrict ourselves to $n = 1$ states and vary μ and R between $1.2 \, \text{GeV}$ and $4 \, \text{GeV}$, which yields order-by-order convergence with moderate perturbative uncertainties. We will perform individual and global fits (for $n = 1$), which are summarized at N^3LO in Fig. 3. We find that the result of the global fit is almost identical to the individual fit to the J/ψ state, due to its extremely precise mass value with respect to the η_c state.

As previously, we take the MSRn scheme as our default, so our final value for the charm quark mass from the global fit of $n = 1$ states is :

$$\overline{m}_c(\overline{m}_c) = 1.273 \pm 0.0005_{\text{exp}} \pm 0.054_{\text{pert}} \pm 0.006_{\alpha_s} \pm 0.0001_{\overline{m}_b} \, \text{GeV} = 1.273 \pm 0.054 \, \text{GeV}. \quad (3.3)$$

Again, we observe that theoretical uncertainties greatly dominate over α_s uncertainties, and again experimental uncertainties (coming form the fit) are negligibly small. The $\overline{m}_b$ uncertainty is also negligible, as the dependence on the bottom mass comes only from the α_s threshold matching from 5 to 4 flavors. A more complete analysis of this work is to be found in Ref. [5].

References

[1] N. Brambilla, A. Pineda, J. Soto and A. Vairo, *Potential NRQCD: An Effective theory for heavy quarkonium*, *Nucl. Phys.* **B566** (2000) 275, [`hep-ph/9907240`].

[2] Y. Kiyo and Y. Sumino, *Full Formula for Heavy Quarkonium Energy Levels at Next-to-next-to-next-to-leading Order*, *Nucl. Phys.* **B889** (2014) 156–191, [`1408.5590`].

[3] N. Brambilla, Y. Sumino and A. Vairo, *Quarkonium spectroscopy and perturbative QCD: A New perspective*, *Phys. Lett.* **B513** (2001) 381–390, [`hep-ph/0101305`].

[4] A. H. Hoang, A. Jain, C. Lepenik, V. Mateu, M. Preisser, I. Scimemi et al., *The MSR Mass and the $\mathcal{O}(\Lambda_{QCD})$ Renormalon Sum Rule*, `1704.01580`.

[5] V. Mateu and P. G. Ortega, *Bottom and Charm Mass determinations from global fits to $Q\bar{Q}$ bound states at N^3LO*, `1711.05755`.

[6] A. A. Penin and M. Steinhauser, *Heavy quarkonium spectrum at $\mathcal{O}(\alpha_s^5 m_q)$ and bottom / top quark mass determination*, *Phys. Lett.* **B538** (2002) 335–345, [`hep-ph/0204290`].

[7] M. Beneke, Y. Kiyo and K. Schuller, *Third-order Coulomb corrections to the S-wave Green function, energy levels and wave functions at the origin*, *Nucl. Phys.* **B714** (2005) 67–90, [`hep-ph/0501289`].

[8] N. Brambilla, Y. Sumino and A. Vairo, *Quarkonium spectroscopy and perturbative QCD: Massive quark loop effects*, *Phys. Rev.* **D65** (2002) 034001, [`hep-ph/0108084`].

[9] Y. Kiyo and Y. Sumino, *Perturbative heavy quarkonium spectrum at next-to-next-to-next-to-leading order*, *Phys. Lett.* **B730** (2014) 76–80, [`1309.6571`].

[10] A. H. Hoang, A. Jain, I. Scimemi and I. W. Stewart, *Infrared Renormalization Group Flow for Heavy Quark Masses*, *Phys. Rev. Lett.* **101** (2008) 151602, [`0803.4214`].

[11] D. Eiras and J. Soto, *Light fermion finite mass effects in non-relativistic bound states*, *Phys. Lett.* **B491** (2000) 101–110, [`hep-ph/0005066`].

[12] A. H. Hoang, *Bottom quark mass from Upsilon mesons: Charm mass effects*, `hep-ph/0008102`.

[13] M. Beneke, A. Maier, J. Piclum and T. Rauh, *The bottom-quark mass from non-relativistic sum rules at NNNLO*, *Nucl. Phys.* **B891** (2015) 42–72, [`1411.3132`].

[14] N. Gray, D. J. Broadhurst, W. Grafe and K. Schilcher, *Three Loop Relation of Quark $\overline{MS}$ and Pole Masses*, *Z. Phys.* **C48** (1990) 673–680.

[15] S. Bekavac, A. Grozin, D. Seidel and M. Steinhauser, *Light quark mass effects in the on-shell renormalization constants*, *JHEP* **10** (2007) 006, [`0708.1729`].

[16] PARTICLE DATA GROUP collaboration, C. Patrignani et al., *Review of Particle Physics*, *Chin. Phys.* **C40** (2016) 100001.

[17] G. D'Agostini, *On the use of the covariance matrix to fit correlated data*, *Nucl. Instrum. Meth.* **A346** (1994) 306–311.

[18] C. Ayala, G. Cvetič and A. Pineda, *The bottom quark mass from the $\Upsilon(1S)$ system at NNNLO*, *JHEP* **09** (2014) 045, [`1407.2128`].