Bottom and charm mass determinations from global fits to $Q\bar{Q}$ bound states at $N^3\text{LO}$

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ABSTRACT: The bottomonium spectrum up to $n = 3$ is studied within Non-Relativistic Quantum Chromodynamics up to $N^3\text{LO}$. We consider finite charm quark mass effects both in the QCD potential and the $\overline{\text{MS}}$ -pole mass relation up to third order in the Υ -scheme counting. The $u = 1/2$ renormalon of the static potential is canceled by expressing the bottom quark pole mass in terms of the MSR mass. A careful investigation of scale variation reveals that, while $n = 1, 2$ states are well behaved within perturbation theory, $n = 3$ bound states are no longer reliable. We carry out our analysis in the $n_\ell = 3$ and $n_\ell = 4$ schemes and conclude that, as long as finite m_c effects are smoothly incorporated in the MSR mass definition, the difference between the two schemes is rather small. Performing a fit to $b\bar{b}$ bound states we find $\bar{m}_b(\bar{m}_b) = 4.216 \pm 0.039 \text{ GeV}$. We extend our analysis to the lowest lying charmonium states finding $\bar{m}_c(\bar{m}_c) = 1.273 \pm 0.054 \text{ GeV}$. Finally, we perform simultaneous fits for $\bar{m}_b$ and α_s finding $\alpha_s^{(n_f=5)}(m_Z) = 0.1178 \pm 0.0051$. Additionally, using a modified version of the MSR mass with lighter massive quarks we are able to predict the uncalculated $\mathcal{O}(\alpha_s^4)$ virtual massive quark corrections to the relation between the $\overline{\text{MS}}$ and pole masses.

KEYWORDS: Quark Masses and SM Parameters, Effective Field Theories, Heavy Quark Physics, Perturbative QCD

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1 Introduction

The precise determination of hadron spectroscopy from fundamental principles pursues to unveil QCD at its non-perturbative regime. The non-perturbative nature of QCD at hadronic scales implied the development of phenomenological approaches such as quark models [1–5] or, more recently, computer-based calculations using Lattice QCD [6–9]. However, the unique properties of heavy quarkonium systems allow an entire calculation in terms of non-relativistic QCD (NRQCD for short) in its weak coupling regime (that is, in pure perturbation theory). Effective Field Theories (EFT for short) provide a clean separation of scales, enabling non-perturbative effects to be either factorized or treated in an Operator Product Expansion. Within perturbative NRQCD the quarkonium masses have been computed in recent years up to N³LO precision, that is up to $\mathcal{O}(m_Q\alpha_s^5)$ and $\mathcal{O}(m_Q\alpha_s^5 \log \alpha_s)$ [10–19]. The development of EFTs such as velocity NRQCD (vNRQCD) [20] and potential NRQCD (pNRQCD) [21, 22], which describe the interactions

of a non-relativistic system with ultrasoft gluons, organizing the perturbative expansions in α_s and the velocity of heavy quarks systematically, has been crucial to reach such accuracy. Finally, a closed expression for arbitrary quantum numbers can be found in ref. [23], which uses mathematical methods to convert infinite sums into finite nested sums and transcendental numbers, and expresses the so called Bethe logarithm as a one-parameter (numerical) integral.

The central object to compute the energy levels of $Q\bar{Q}$ states¹ is the QCD color-singlet static potential $V_{\text{QCD}}(r)$, which is known to very high accuracy: the leading correction, $\mathcal{O}(\alpha_s)$ with respect to the Coulomb term, was obtained in [10], the $\mathcal{O}(\alpha_s^2)$ terms were computed in refs. [12, 24], while the $\mathcal{O}(\alpha_s^3)$ corrections were calculated in refs. [14, 17–19, 25]. It is well understood that the QCD static potential suffers from an $\mathcal{O}(\Lambda_{\text{QCD}})$ renormalon ambiguity that exactly cancels that of the pole mass [26–28], such that the static energy $E_{\text{stat}}(r) = 2m_Q^{\text{pole}} + V_{\text{QCD}}(r)$ is renormalon free.² This cancellation is essential to make the energy levels of quarkonia perturbative objects. For this cancellation to take place, the pole mass has to be expressed in terms of so called short-distance masses. Previous studies of the bottomonium and charmonium spectra used the renormalization-scale-dependent $\overline{\text{MS}}$ mass $\bar{m}_Q(\mu)$ evaluated at $\mu = \bar{m}_Q$ [29–31]. Although this scheme will make the renormalon cancellation happen, it introduces a conceptual (and many times also practical) problem. In the pole scheme, perturbative logs appearing in the theoretical expression of the quarkonium energy levels have the following form: $\log[n\mu/(C_F\alpha_s m_Q)]$, with n the principal quantum number. When expressing the pole mass in terms of $\bar{m}_Q(\bar{m}_Q)$ a new class of logs appear, namely $\log(m_Q/\mu)$.³ It is clear that no single choice of the scale μ will cause both logs to vanish simultaneously. The origin of this mismatch can be traced to the fact that in NRQCD the mass of the heavy quark is a hard scale which has been integrated out. This situation is resolved if instead a low-scale short-distance mass is used, such that the logs introduced when switching scheme either have the form $\log(\mu/R)$, being R an arbitrary scale the mass depends on (MSR mass [32, 33], Potential Subtracted (PS) mass [28], Renormalon Subtracted mass (RS) [34], kinetic mass [35] or jet mass [36, 37]), which can be chosen of the same order as (or equal to) μ , or they are already of the exact same form as the original ones (1S mass [38–40]). While the recent analysis of ref. [41] employs the RS mass, we will make use of the MSR mass, motivated by the fact that it is straightforward to include effects of lighter massive quarks [42].⁴ At this point a comment is in order: while the problem just described is indeed critical for the top quark, it is a lot less severe for the bottom and charm quarks, given that the hierarchy between their masses and the respective non-relativistic scales is not very large. It is nevertheless theoretically more sound to use a low-scale mass.

¹In the rest of the paper Q will stand for the heavy, non-relativistic quark forming the bound states, while q will refer to the next lighter quark.

²For this cancellation to happen it is essential that the ambiguity of the pole mass and the potential are independent of the mass and r , respectively.

³In practice these logs are present because even if the $\overline{\text{MS}}$ mass is evaluated at the scale $\mu = \bar{m}_Q$, the relation of the pole mass to $\bar{m}_Q(\bar{m}_Q)$ has to be written as a series in powers of $\alpha_s(\mu)$ for the renormalon cancellation to take place.

⁴Here we will use a modified version of the MSR mass in which the effects of virtual massive quarks participate in the R-evolution.

The last piece needed to assemble the complete N³LO theoretical expression in a short-distance scheme is the four-loop coefficient of the relation between the $\overline{\text{MS}}$ and pole masses, which has been computed recently [43, 44]. This term is necessary to compute the MSR mass to the same accuracy as the static potential in the so called Υ -expansion scheme [38, 39]. To make the list of theoretical ingredients complete one needs to include the effects of the finite charm mass both in the static potential and the $\overline{\text{MS}}$ to pole mass relation. Both are known up to $\mathcal{O}(\varepsilon^3)$: at two [45] and three [46] loops for the latter; for any state at two loops [47] and for $n = 1$ states at three loops [48], for the former. Therefore, if we are to include charm quark mass effects in the static potential, we have to include them in the MSR mass as well. The MSR mass has so far been used only in phenomenological applications up to $\mathcal{O}(\alpha_s)$, and always in the context of jet physics [49, 50]. One (theoretical) motivation of our study is thus employing the MSR mass at $\mathcal{O}(\alpha_s^4)$ and in the context of a non-relativistic system. Furthermore, we want to test how efficiently the MSR mass deals with lighter massive flavors in a practical application.

Comparing the theoretical predictions for the bottomonium and charmonium masses with the corresponding experimental values one can determine the bottom and charm quark masses with good accuracy in a clean environment. Precise values of these heavy quark masses are key to test the validity of the Standard Model in the precision frontier, both in Flavor [51] and Higgs Physics [52]. Two recent analyses have determined the bottom quark mass from the $\Upsilon(1S)$ state [41],⁵ and bottom and charm quark masses from $n = 1$ states [54]. Both analyses use N³LO theoretical predictions and consider finite charm quark mass corrections. While [41] uses the RS scheme for the heavy quark mass and varies μ and R independently (but one at a time) in a non-relativistic range (1.5 GeV to 4 GeV), ref. [54] uses the $\overline{\text{MS}}$ scheme and the principle of minimal sensitivity, setting μ at scales that are larger than the heavy quark mass itself (5 GeV to 12 GeV for bottom, 2 GeV to 4.5 GeV for charm), therefore relativistic. In our analysis we will use the MSR scheme varying both renormalization scales independently and simultaneously around the value that minimizes perturbative logarithms (a non-relativistic scale). Additionally, based on the observation made in ref. [30], that is, finite charm quark mass effects in bottomonium are closer to the decoupling ($m_c \rightarrow \infty$) than to the massless ($m_c \rightarrow 0$) limit, the authors of ref. [41] argue that using $n_\ell = 3$ active flavors makes this decoupling more explicit, and therefore carry out their analysis in this scheme. On the other hand, ref. [54] performs the bulk of their analysis in the $n_\ell = 4$ flavor scheme, and uses its difference to the $n_\ell = 3$ result to estimate the uncertainties due to missing higher terms on the finite charm mass correction. We perform fits in both flavor schemes but take the $n_\ell = 3$ determination for our final result.

The main motivation to carry out our analysis is to include in the determination of the bottom quark mass states with principal quantum number $n \geq 1$. It has been claimed that the gross spectrum of bottomonium up to $n = 4$ can be described purely within perturbation theory [29–31]. Those analyses are based on the $\overline{\text{MS}}$ scheme for the bottom quark and on the principle of minimal sensitivity to the renormalization scale,

⁵See [53] for an update of the analysis.

which in practice translates into settings the scale μ far from the (low energy) values that would make perturbative logarithms vanish, and vary it in a very narrow range or towards larger scales. We shall show that the scale of minimal sensitivity strongly depends on the order of perturbation theory considered, and also on the ℓ, s and j quantum numbers which do not appear in the perturbative logarithms. We perform a dedicated study of scale variation inspired by the usual lore, that is, the argument of perturbative logarithms should vary roughly between $1/2$ and 2 , supplemented with the additional constraint that the renormalization scale should not become smaller than 1 GeV , such that perturbation theory is not jeopardized. We find that the central renormalization scale decreases as n increases, becoming smaller than 1 GeV already at $n = 3$. Even stopping scale variation at 1 GeV for $n = 3$, the predictions for the masses become unstable and the perturbative uncertainties grow dramatically as compared to smaller values of n .

Our analysis would not be complete if non-perturbative effects are simply ignored.⁶ We will assume that the soft scale mv is much larger than Λ_{QCD} , and that the ultra-soft scale mv^2 is either much larger than Λ_{QCD} , or at the very worst, of the same order. The analysis of ref. [55] suggests that for states with $n = 1$ we are in the former situation (therefore non-perturbative effects come in the form of local condensates), while for $n = 2$ likely falls in the latter (with non-perturbative effects manifesting themselves as non-local condensates). In either situation the main contribution to the energy levels is perturbation theory. Our analysis seems to indicate that for $n \geq 3$ one has $mv^2 < \Lambda_{\text{QCD}}$, being the static potential directly affected by non-local condensates. Our approach to non-perturbative effects will be rather heuristic: given that the operator product expansion ties together perturbative and non-perturbative physics, we will assume that as long as the perturbative expansion for the energy levels is well behaved, non-perturbative effects do not heavily affect the perturbative result. We will give extra validation to this ansatz by comparing the determination of the bottom quark mass from fits to states with principal quantum numbers $n = 1$ and $n = 2$. From this analysis we can however not discard that for $n = 2$ we are already in a situation in which perturbative and non-perturbative effects become entangled, and until a fully fledged study of non-perturbative effects becomes available, it is not possible to draw further conclusions. As emphasized in ref. [41], one probably needs to have ultrasoft effects under control before dealing with non-perturbative physics.

This article is organized as follows: in section 2 we provide the theoretical expressions for quarkonia masses including corrections from massive lighter quarks. In section 3 we review the MSR short-distance scheme for the mass of a heavy quark and show how to include effects from massive lighter quarks in their R-evolution, explaining how to integrate those effects out at low scales. In section 4 we perform an investigation of renormalization scale variation and the effects of finite charm mass in bottomonium. The fitting procedure and the results for the determination of the bottom and charm quark masses, as well as simultaneous fits to $\overline{m}_b$ and α_s , are presented in section 5. We compare our results to previous determinations in section 6. Our conclusions are contained in section 7. Some formulas are collected in appendix A.

⁶We thank Thomas Rauh for bringing our attention to this issue.

2 Formula for $Q\bar{Q}$ bound states

2.1 Analytic expression for massless quarks

The energy of a $Q\bar{Q}$ non-relativistic bound state characterized by the (n, j, ℓ, s) quantum numbers and with n_ℓ massless active flavors reads in the pole scheme [16, 23, 56]:

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

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

with H_n the harmonic number. In Eq (2.1) ε is a bookkeeping parameter that labels the various orders in the Υ -expansion. The $c_{i,j}$ coefficients can be computed from the $c_{i,0}$ imposing μ independence of the energy states, what implies the following recursion relation:

$$c_{k,j+1} = \frac{2}{j+1} \left\{ (j+2) \beta_{k-1-j} c_{j,j} + \sum_{i=j+1}^{k-1} \beta_{k-1-i} [(i+2) c_{i,j} - (j+1) c_{i,j+1}] \right\}, \quad (2.2)$$

where β_i are the $(i+1)$ -loop coefficients of the beta function defined in eq. (3.2). The $c_{i,0}$ coefficients have been calculated up to $i=3$ and their values can be found in refs. [30, 31]. In general they depend on the quantum numbers (n, j, ℓ, s) and $c_{3,0}$ also depends on $\log(\alpha_s)$. Eq. (2.1) inherits the $u=1/2$ renormalon of the static potential, what makes it unfit for a precision determination of heavy quark masses. This can be resolved by expressing the pole mass in terms of a short-distance mass. Moreover, if large logs of the ratio of the non-relativistic scale and the quark mass are to be avoided, a low-scale short-distance mass should be used. In our analysis we employ the two versions of the MSR mass discussed in ref. [33]. Let us consider a generic short-distance mass whose relation to the pole scheme is expressed as

$$m_Q^{\text{pole}} = m_Q^{\text{SD}} \left[1 + \sum_{n=1} \varepsilon^n \delta_n^{\text{SD}} \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^n \right], \quad (2.3)$$

where m_Q^{SD} depends on some energy scale denoted generically by R , and δ_n^{SD} contain powers of $\log(\mu/R)$. One then has that

$$L_{n_\ell} = L_{\text{SD}} - \sum_{i=1} \varepsilon^i \delta_i^L \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i, \quad L_{\text{SD}} = \log \left(\frac{n\mu}{C_F \alpha_s^{(n_\ell)}(\mu) m_Q^{\text{SD}}} \right) + H_{n+\ell},$$

$$\delta_{i+1}^L = \delta_{i+1}^{\text{SD}} - \frac{1}{i+1} \sum_{j=1}^i j \delta_j^L \delta_{i+1-j}^{\text{SD}}. \quad (2.4)$$

This relation can be used to convert the sum that appears in eq. (2.1) to a short-distance scheme:

$$\begin{aligned}
 \sum_{i=0}^{\infty} \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i \varepsilon^{i+1} P_i(L_{n_\ell}) &= \sum_{i=0}^{\infty} \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i \varepsilon^{i+1} P_i^{\text{SD}}(L_{\text{SD}}), \\
 P_j^{\text{SD}} &= \sum_{i=1}^{j+1} \sum_{k=0}^{\min(i-1, j+1-i)} c_{i,k}^{\text{SD}} \delta_{k,j+1-i}^L, \\
 c_{i,k}^{\text{SD}} &= (-1)^k \sum_{j=k}^{i-1} \binom{j}{k} c_{i,j} L_{\text{SD}}^{j-k}, \\
 \delta_{1,i}^L &= \delta_i^L, \quad \delta_{n+1,j}^L = \sum_{i=1}^{j-n} \delta_i^L \delta_{n,j-i}^L.
 \end{aligned} \tag{2.5}$$

Here we have defined the $\delta_{i,j}^L$ coefficients from $(\sum_{i=1} x^i \delta_i^L)^j = \sum_{i=j} x^i \delta_{j,i}^L$, which can be calculated from the recursion relation in the last line of eq. (2.5). The only thing left to express the energy levels of quarkonium in a short-distance scheme is converting the global factor m_Q^{pole} :

$$\begin{aligned}
 E_X(\mu, n_\ell) &= 2 m_Q^{\text{SD}} \left\{ 1 + \sum_{i=1} \varepsilon^i \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i \left[\delta_i^{\text{SD}} - F P_{i-1}^{\text{SD}} - (1 - \delta_{i,1}) F \sum_{j=1}^{i-1} \delta_j^{\text{SD}} P_{i-j-1}^{\text{SD}} \right] \right\}, \\
 F &= \frac{\pi C_F^2 \alpha_s^{(n_\ell)}(\mu)}{2n^2},
 \end{aligned} \tag{2.6}$$

where $\delta_{1,i}$ is the Kronecker symbol taking the value 1 for $i = 1$ and zero for higher values of i .

Having in mind that ultimately we want to determine the mass of the heavy quark Q , one can devise perturbative expansions based on eq. (2.6) in which m_Q^{SD} (or even $\bar{m}_Q$) is singled out. We use two such expansions, which are in complete correspondence to the “linearized” and “linearized iterative” methods defined in ref. [57], and denote them as *expanded out* and *iterative*. The former corresponds to:

$$m_Q^{\text{SD}} = \frac{E_X^{\text{exp}}}{2} \left[1 + \sum_{i=1} \varepsilon^i \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i A_i^{\text{exp}}(m_Q^{\text{SD}}, R, \mu,) \right], \tag{2.7}$$

directly obtained from eq. (2.6) isolating the global factor m_Q^{SD} , with E_X^{exp} the experimental value for the bound state and A_i^{exp} some easy-to-calculate coefficients. One can remove the m_Q^{SD} dependence that still persists on the A_i^{exp} in an iterative way, by introducing lower-order expressions for m_Q^{SD} in higher-order ones and expanding consistently in ε . This way one obtains the iterative expansion:

$$m_Q^{\text{SD}} = \frac{E_X^{\text{exp}}}{2} \left[1 + \sum_{i=1} \varepsilon^i \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^i A_i^{\text{iter}}(E_X^{\text{exp}}, R, \mu,) \right]. \tag{2.8}$$

There is still some residual m_Q dependence on the right hand side due to the threshold matching conditions of α_s . This can be eliminated numerically by iterating eq. (2.8) a few times.

2.2 Finite charm mass effects on bottomonium

Equation (2.1) considers that the n_ℓ active flavors that contribute to the energy of a $Q\bar{Q}$ bound state are all massless. However, massive charm quark loops contribute both to the binding energy and the relation of the pole and short-distance masses, which should be properly accounted for. In this section we consider both m_Q m_q in the pole scheme, since switching any of them to a short-distance scheme is trivial. Whenever we use a short-distance scheme for m_Q , we will take m_q in the $\overline{\text{MS}}$ scheme, and more specifically we will only use $\bar{m}_q \equiv \bar{m}_q^{(n_\ell)}(\bar{m}_q^{(n_\ell)})$. Massive lighter quarks effects on the relation between the pole and other short-distance schemes will be discussed in sections 3.2, 3.3 and 3.4.

Modifications to the Coulomb potential due to non-zero lighter quark masses have been calculated up to $\mathcal{O}(\varepsilon^3)$. The direct consequence of such corrections in the Coulomb potential is an energy-shift effect in the heavy quarkonium mass. In the pole scheme they read:

$$E_X(\mu, n_\ell, m_Q^{\text{pole}}, m_q^{\text{pole}}) = E_X(\mu, n_\ell, m_Q^{\text{pole}}) + \varepsilon^2 \delta E_X^{(1)} + \varepsilon^3 \delta E_X^{(2)}. \quad (2.9)$$

If eq. (2.9) is expressed in the n_ℓ scheme, where the massless limit is realized, these corrections obviously vanish if $m_q \rightarrow 0$. Likewise, if eq. (2.9) is written in the $(n_\ell - 1)$ scheme, the decoupling limit is realized and the corrections should vanish if $m_q \rightarrow \infty$. However, in the $n_\ell (n_\ell - 1)$ scheme the decoupling (massless) limit is not manifest. We can use this information to constrain the form of $\delta E_X^{(i)}$ in the n_ℓ scheme for large values of m_q requiring that, once $\alpha_s^{(n_\ell)}$ is expressed in terms $\alpha_s^{(n_\ell-1)}$ through the threshold relation in eq. (3.9) the decoupling limit is reached. This strategy was used in ref. [30].

The ε^2 correction has been calculated in ref. [47], for arbitrary quantum numbers, and in the n_ℓ scheme it reads:

$$\begin{aligned} \delta E_X^{(1)}(n_\ell) &= \alpha_s^{(n_\ell)}(\mu)^3 \delta E_1(\rho), \\ \delta E_1(\rho) &= \frac{C_F^2}{3(4\pi)n^2} \left[-\frac{1}{(2n-1)!} \sum_{k=0}^{n-\ell-1} \binom{n-\ell-1}{k} \binom{n+\ell}{k+2\ell+1} \rho^{2(n-k-\ell-1)} f_D(n, \ell, k, \rho) \right. \\ &\quad \left. - \pi n \rho^3 \left((n-\ell-1)(n+\ell) + \frac{1}{3}(n+1)(2n+1) \right) + \rho^2 \left((n-\ell-1)(n+\ell) + (2n+1)n \right) \right. \\ &\quad \left. - \frac{3\pi}{2} n \rho + 2 \ln \left(\frac{2}{\rho} \right) - 2 H_{n+\ell} \right], \end{aligned} \quad (2.10)$$

where $\rho = (2n m_c)/[m_b C_F \alpha_s^{(n_\ell)}(\mu)]$ and $f_D(n, \ell, k, \rho)$ is defined in eq. (A.1). In the $(n_\ell - 1)$ scheme one simply has

$$\delta E_X^{(1)}(n_\ell - 1) = \alpha_s^{(n_\ell-1)}(\mu)^3 \left[\delta E_1(\rho) - \lim_{\rho \rightarrow \infty} \delta E_1(\rho) \right], \quad (2.11)$$

such that the decoupling limit is manifest.

The exact $\mathcal{O}(\varepsilon^3)$ finite charm mass corrections to the binding energy have been computed for the $n = 1$ bottomonium energy levels in ref. [48], and for states with arbitrary n and $\ell = 0$ in ref. [58], remaining unknown for other sets of quantum numbers. Since these

Figure 1. Finite charm quark mass corrections to the $\Upsilon(1S)$ mass at $\mathcal{O}(\varepsilon^3)$ in the pole scheme. We take the values $m_b = 4.2$ GeV, $\mu = 2$ GeV and $\alpha_s^{(n_f=5)}(m_Z) = 0.118$. The blue line corresponds to the exact result, while the red solid line is the approximation described in the text. The red dashed line shows the decoupling limit approximation.

corrections for $n > 1$ are prohibitively slow, in order to include them for non- $1S$ states we will use the results of the analysis carried out in ref. [30], where the authors concluded that for $n = 1$ the $m_c \rightarrow \infty$ limit is an excellent approximation, which becomes even better for large values of the principal quantum number. The formula for such limit in the pole mass scheme is detailed in eq. (A.2). We will supplement this approximation with the requirement that in the n_ℓ scheme the correction must vanish if $m_c \rightarrow 0$. Our approach uses the decoupling approximation for values of m_c larger than $m_c^*(n)$, where $m_c^*(n) = (1 \text{ GeV})/\sqrt{n}$, and the fit function $f(m_c) = m_c [a + b \log(m_c)]$ for $m_c < m_c^*$, where the coefficients a and b are adjusted such that the transition is smooth at the junction point. This functional form enforces the massless limit, and the dependence of m_c^* in n takes the decoupling approximation as exact for lower values of m_c . We have tested our approach for $n = 1$ and found that it reproduces the exact known result within a few percent, as can be appreciated in figure 1. In this figure we also show the decoupling approximation below the junction point as a red dashed line.

3 The MSR scheme

As mentioned in the Introduction, the use of the pole mass in perturbative calculations is ineffective, not only for its bad perturbative behavior but also because of the existence of confinement, which hides the quark propagator pole in the non-perturbative regime.

Alternatively, the $\overline{\text{MS}}$ mass is an adequate scheme for physical situations that involve energies much larger than the heavy quark. Ideally, for the heavy quarkonium, one would like to extend such scheme for energies below m_Q without losing the good infrared properties of the $\overline{\text{MS}}$ scheme. At such scales the evolution of the logarithms in the regular $\overline{\text{MS}}$ mass is unphysical and behaves badly. A more adequate short-distance scheme is the MSR mass. The MSR scheme, first introduced in ref. [32], and extensively discussed in

ref. [33], is a natural extension of the $\overline{\text{MS}}$ mass for renormalization scales below the heavy quark mass. The definition of the MSR mass, expressed as the MSR-pole mass difference, is derived directly from the $\overline{\text{MS}}$ pole mass relation, exploiting the fact that the renormalon ambiguity is independent of the value of the heavy quark mass. Let us start from the perturbative relation of the $\overline{\text{MS}}$ and pole masses:

$$\delta \overline{m}_Q(\overline{m}_Q) \equiv m_Q^{\text{pole}} - \overline{m}_Q = \overline{m}_Q \sum_{n=1}^{\infty} a_n^{\overline{\text{MS}}}(n_\ell, n_h) \left(\frac{\alpha_s^{(n_\ell+n_h)}(\overline{m}_Q)}{4\pi} \right)^n, \quad (3.1)$$

where $n_f = n_\ell + n_h$ and we have defined $\overline{m}_Q \equiv \overline{m}_Q^{(n_f)}(\overline{m}_Q^{(n_f)})$. The strong coupling constant is expressed in the $\overline{\text{MS}}$ scheme with the usual renormalization group equation:

$$\frac{d\alpha_s^{(n_f)}(\mu)}{d \ln \mu} = -2 \alpha_s^{(n_f)}(\mu) \sum_{n=0}^{\infty} \beta_n(n_f) \left(\frac{\alpha_s^{(n_f)}(\mu)}{4\pi} \right)^{n+1}. \quad (3.2)$$

For later use we split the two- and three-loop terms into their various flavor components

$$\begin{aligned} a_2^{\overline{\text{MS}}} &= a_2^{(g)} + n_\ell a_2^{(n_\ell)} + n_h a_2^{(n_h)}, \\ a_3^{\overline{\text{MS}}} &= a_3^{(g)} + n_\ell a_2^{(n_\ell)} + n_h a_2^{(n_h)} + n_\ell^2 a_2^{(n_\ell^2)} + n_h^2 a_2^{(n_h^2)} + n_\ell n_h a_2^{(n_\ell n_h)}. \end{aligned} \quad (3.3)$$

In contrast to the $\overline{\text{MS}}$ mass, which only depends logarithmically in the scale μ , the MSR mass has a logarithmic and linear dependence on R :

$$\begin{aligned} \delta m_Q^{\text{MSR}} \equiv m_Q^{\text{pole}} - m_Q^{\text{MSR}}(R) &= R \sum_{n=1}^{\infty} a_{n,0}(n_\ell) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^n \\ &= R \sum_{n=1}^{\infty} \sum_{k=0}^n a_{n,k}(n_\ell) \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^n \ln^k \left(\frac{\mu}{R} \right), \end{aligned} \quad (3.4)$$

where $a_{n,k}$ are derived from eq. (3.1), and are different for the Practical and Natural versions of the MSR mass (see section 3.1). The advantages of this mass scheme is that it can be safely employed for scales $R < m_Q$ when a clean treatment of virtual massive-quark effects is relevant, as the virtual effects of the massive flavor is integrated out from the MSR mass expression.

While the first line of eq. (3.4) defines the MSR mass and is used to derive its anomalous dimension, the second line is more useful when implementing the MSR scheme in a series expressed in powers of $\alpha_s(\mu)$. Since the MSR mass is μ -independent, the $a_{n,k}$ coefficients can be computed from the $a_{k,0}$ with the following recursion relation:

$$a_{n,k} = \frac{2}{k} \sum_{i=k}^{n-1} i a_{i,k-1} \beta_{n-1-i}. \quad (3.5)$$

The R dependence of the MSR mass is described by the following renormalization group equation:

$$-\frac{d}{dR} m_Q^{\text{MSR}}(R) = \gamma^R[\alpha_s^{(n_\ell)}(R)] = \sum_{n=0}^{\infty} \gamma_n^R \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^{n+1}, \quad (3.6)$$

where γ_n^R are the R-anomalous dimension coefficients [33], which can be calculated as follows:

$$\gamma_n^R = a_{n+1,0} - 2 \sum_{j=0}^{n-1} (n-j) \beta_j a_{n-j,0}. \quad (3.7)$$

Since the ambiguity of eq. (3.4) is R independent, the R-anomalous dimension is automatically renormalon-free. This RGE provides a systematic reordering of the terms in the asymptotic series related to the $\mathcal{O}(\Lambda_{\text{QCD}})$ renormalon ambiguity:

$$m_Q^{\text{MSR}}(R_2) - m_Q^{\text{MSR}}(R_1) = \int_{R_1}^{R_2} dR \gamma_n^R[\alpha_s^{(n_\ell)}(R)], \quad (3.8)$$

which results in the summation of powers of $\log(R_1/R_0)$ to all orders in perturbation theory.⁷

3.1 Natural and practical MSR schemes

As we discussed in section 3, in contrast to the $\overline{\text{MS}}$ mass, the MSR mass is a suitable scheme for applications requiring scales lower than the heavy quark mass. For that reason, the UV effects of the quark Q can be integrated out, changing from a scheme with $n_\ell + 1$ dynamical flavors to one with only n_ℓ . There are, hence, two alternative but equivalent ways to achieve this transformation. On the one hand, the threshold matching relation for the strong coupling can be used to rewrite $\alpha_s^{(n_\ell+1)}$ in terms of $\alpha_s^{(n_\ell)}$

$$\alpha_s^{(n_\ell+1)}(\overline{m}_Q) = \alpha_s^{(n_\ell)}(\overline{m}_Q) \left[1 + \sum_{n=2} \xi_n(n_\ell) \left(\frac{\alpha_s^{(n_\ell)}(\mu)}{4\pi} \right)^n \right], \quad (3.9)$$

which once implemented into eq. (3.1) is used to define the *Practical MSR mass*:

$$m_Q^{\text{pole}} - m_Q^{\text{MSRp}}(R) = R \sum_{n=1}^{\infty} a_n^{\text{MSRp}}(n_\ell) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^n. \quad (3.10)$$

The a_n^{MSRp} coefficients can be computed as follows:

$$a_{n,0}^{\text{MSRp}}(n_\ell, n_h) = \sum_{i=1}^n a_i^{\overline{\text{MS}}}(n_\ell, n_h) \xi_{i-1,n}(n_\ell), \quad (3.11)$$

where we have included the n_h argument in the MSRp scheme coefficients for later convenience. The coefficients $\xi_{i,j}$ are defined as $(1 + \sum_{j=1} \xi_j x^j)^i = 1 + \sum_{j=1} \xi_{i,j} x^j$, and therefore fulfill $\xi_{1,i} = \xi_i$, where we define $\xi_0 = \xi_{i,0} = 1$. For $i > 1$ they can be computed with the following recursion relation:

$$\xi_{n+1,j}(n_\ell) = \xi_j(n_\ell) + \xi_{n,j}(n_\ell) + \sum_{i=1}^{j-1} \xi_i(n_\ell) \xi_{n,j-i}(n_\ell). \quad (3.12)$$

⁷This class of logarithms was first summed up for the RS mass in [59] through the inverse Borel transform of the asymptotic series.

On the other hand, the virtual loop corrections of the heavy quark Q can be directly integrated out of the $\overline{\text{MS}}$ to pole relation taking $n_h = 0$ in eq. (3.1), which leads to the definition of the *Natural MSR mass*:

$$m_Q^{\text{pole}} - m_Q^{\text{MSRn}}(R) = R \sum_{n=1}^{\infty} a_n^{\overline{\text{MS}}}(n_\ell, 0) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^n, \quad (3.13)$$

that is, $a_{n,0}^{\text{MSRn}}(n_\ell) \equiv a_n^{\overline{\text{MS}}}(n_\ell, 0)$.

Each materialization of the $\{n_\ell + 1 \rightarrow n_\ell\}$ scheme change has its advantages, depending on the specific applications. The Natural MSR mass only exhibits corrections arising from gluons and massless quarks, being its relation with the $\overline{\text{MS}}$ mass mediated by a non-trivial expression:

$$m_Q^{\text{MSRn}}(\overline{m}_Q) - \overline{m}_Q = \text{HQS}(\overline{m}_Q, n_\ell, 1), \quad (3.14)$$

$$\text{HQS}(\overline{m}_Q, n_\ell, n_h) \equiv \overline{m}_Q \sum_{n=2} \left[a_k^{\text{MSRp}}(n_\ell, n_h) - a_k^{\overline{\text{MS}}}(n_\ell, n_h - 1) \right] \left(\frac{\alpha_s^{(n_\ell)}(\overline{m}_Q)}{4\pi} \right)^n.$$

Alternatively, the MSRp- $\overline{\text{MS}}$ relation is more direct, as the Practical MSR mass is equal to the $\overline{\text{MS}}$ mass at the scale of the mass to all orders in perturbation theory:

$$m_Q^{\text{MSRp}}(\overline{m}_Q) = \overline{m}_Q(\overline{m}_Q). \quad (3.15)$$

Finally, we note that the $\overline{\text{MS}}$ scheme used in refs. [29–31] exactly corresponds to the MSRp mass with $R = \overline{m}$. Therefore their theoretical expressions are contained in ours.

3.2 $\overline{\text{MS}}$ mass with light fermion masses

Corrections from massive lighter quarks modify the relation of the pole mass to other short-distance schemes. In this section we shall focus the discussion to the $\overline{\text{MS}}$ mass, though for our numerical analysis the MSR scheme will be used.

The corrections from massive lighter quarks to the $\overline{\text{MS}}$ -pole mass relation start at $\mathcal{O}(\alpha_s^2)$ and vanish in the $m_q \rightarrow 0$ limit. Hence the corrected relation can be expressed as:

$$m_Q^{\text{pole}} - \overline{m}_Q \equiv \delta m_Q(\overline{m}_Q) + \overline{m}_Q \Delta_{\overline{m}_c}^{\overline{\text{MS}}}(\overline{m}_Q, \xi), \quad (3.16)$$

$$\Delta_{\overline{m}_c}^{\overline{\text{MS}}}(\overline{m}_Q, \xi) = \sum_{n=2} \left(\frac{\alpha_s^{(n_\ell+n_h)}(\overline{m}_Q)}{4\pi} \right)^n \Delta_n^{\overline{\text{MS}}}(n_\ell, n_h, \xi),$$

where δm_Q is given in eq. (3.1) and $\xi = \overline{m}_q/\overline{m}_Q$. The functions Δ_i obey two constraints: $\Delta_n^{\overline{\text{MS}}}(n_\ell, n_h, 0) = 0$ and $\Delta_n^{\overline{\text{MS}}}(n_\ell, n_h, 1) = a_n^{\overline{\text{MS}}}(n_\ell - 1, n_h + 1) - a_n^{\overline{\text{MS}}}(n_\ell, n_h)$.⁸ The ε^2 term for the non-zero charm mass corrections has been calculated exactly in ref. [45]:⁹

$$\Delta_2^{\overline{\text{MS}}}(\xi) = \frac{16}{3} \left[\ln^2(\xi) + \frac{\pi^2}{6} - \xi^2 \left(\frac{3}{2} + \ln(\xi) \right) + (1+\xi)(1+\xi^3) \left(\text{Li}_2(-\xi) - \frac{1}{2} \ln^2(\xi) + \ln(\xi) \ln(1+\xi) + \frac{\pi^2}{6} \right) - (1-\xi)(1-\xi^3) \left(\frac{\pi^2}{6} + \frac{1}{2} \ln^2(\xi) + \text{Li}_2(1-\xi) \right) \right]. \quad (3.17)$$

⁸These relations will be refereed to as “the $\xi = 0$ constraint” and “the $\xi = 1$ constraint”, respectively, in the rest of the paper.

⁹Eq. (3.17) is written in a way in which each term is manifestly real for any value of ξ between 0 and 1.

This correction, together with its linear approximation [see eq. (3.24)], are shown in figure 3c. The $\xi = 1$ constraint in these corrections takes the form $\Delta_2(1) = a_2^{(n_h)} - a_2^{(n_\ell)}$. The ε^3 correction can be split in three contributions:

$$\Delta_3^{\overline{\text{MS}}}(\xi)(n_\ell, n_h, \xi) = \Delta_3^{(g)}(\xi) + n_\ell \Delta_3^{(n_\ell)}(\xi) + n_h \Delta_3^{(n_h)}(\xi). \quad (3.18)$$

The $\xi = 1$ constraint can be decomposed in the following relations:

$$\begin{aligned} \Delta_3^{(g)}(1) &= a_3^{(n_\ell^2)} + a_3^{(n_h^2)} + a_3^{(n_h)} - a_3^{(n_\ell)} - a_3^{(n_\ell n_h)}, \\ \Delta_3^{(n_\ell)}(1) &= a_3^{(n_\ell n_h)} - 2 a_3^{(n_\ell^2)}, \\ \Delta_3^{(n_h)}(1) &= 2 a_3^{(n_h^2)} - a_3^{(n_\ell n_h)}. \end{aligned} \quad (3.19)$$

The exact expression for $\Delta_3^{(g, n_\ell, n_h)}$ has been analytically calculated in ref. [46], but it is terribly lengthy, therefore impractical for a numerical implementation. Ref. [46] provides 8 terms of the expansion for small ξ , which can be combined with the $\xi = 1$ constraint in a Padé parametrization to provide an approximation which is accurate to 8 significant digits across the range $0 \leq \xi \leq 1$, which is enough for our purposes. Our parametrizations are explicitly shown in eq. (A.3). In figure 3a $\Delta_3^{\overline{\text{MS}}}(\xi)(n_\ell = 4, n_h = 0, \xi)$ is shown, together with the approximation given in eq. (3.25).

3.3 MSR mass with light active fermion masses

To include effects from lighter massive quarks we follow the same approach that was used in ref. [60] to implement R-evolution in the gap parameter of the soft function when secondary heavy quarks are produced through gluon splitting. This implementation in the MSR mass happens to satisfy Heavy Quark Symmetry (HQS for short) exactly. HQS states that in the limit of an infinitely heavy quark, low-energy QCD effects are flavor independent. This limit has to be taken only in the virtual effects, as only quantum fluctuations are integrated out. If one looks into $m_Q^{\text{pole}} - m_Q^{\overline{\text{MS}}}$ in this limit, n_h becomes 0, what effectively converts this series to the MSRn scheme, and m_q/m_Q tends to 0, what makes the lighter q quark massless. For $m_q^{\text{pole}} - m_q^{\overline{\text{MS}}}$ one has that $m_q \rightarrow 0$ in the virtual effects implies $n_h \rightarrow 0$ and $n_\ell - 1 \rightarrow n_\ell$. Therefore in this limit $m_Q^{\text{pole}} - m_Q^{\text{MSRn}}(\overline{m}_q) = m_q^{\text{pole}} - m_q^{\overline{\text{MS}}}$. With our definition this equality will be satisfied even for finite values of the heavy quark mass. Although there is no theoretical advantage in having (for the MSRn mass) heavy quark symmetry (accidentally) exact, and the impact of this feature in the final results is small, it has a practical advantage, as it ensures a smooth transition to an MSR mass in which the lighter quark q is also integrated out.

Our definition of the MSR mass including non-zero lighter quark masses reads:¹⁰

$$\delta m_Q^{\text{MSR}}(R, \bar{m}_q) = \delta m_Q^{\text{MSR}}(R) + R \Delta_{\bar{m}_q}(R, \xi_R), \quad (3.20)$$

$$\Delta_{\bar{m}_q}(R, \xi_R) = \sum_{k=2} \Delta_{\bar{m}_q}^{(k)}(\xi_R) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^k,$$

where $\xi_R = \bar{m}_q/R$. In the MSRn scheme one has $\Delta_{\bar{m}_q}^{(n)} = \Delta_n^{\overline{\text{MS}}}|_{n_h=0}$. For the MSRp scheme, at two loops one has $\Delta_{\bar{m}_q}^{(2)} = \Delta_2^{\overline{\text{MS}}}$ and at three loops $\Delta_{\bar{m}_q}^{(3)} = \Delta_3^{\overline{\text{MS}}}|_{n_h=1}$ (nontrivial modifications in the MSRp scheme start at 4 loops). The nice property of eq. (3.20) is that in the case of the MSRn scheme one has exact Heavy Quark Symmetry:

$$\begin{aligned} m_Q^{\text{pole}} - m_Q^{\text{MSRn}}(\bar{m}_q) &= \bar{m}_q \sum_{n=1} \left[a_n^{\overline{\text{MS}}}(n_\ell, 0) + \Delta_n^{\overline{\text{MS}}}(n_\ell, 0, 1) \right] \left(\frac{\alpha_s^{(n_\ell)}(\bar{m}_q)}{4\pi} \right)^n \\ &= \bar{m}_q \sum_{n=1} a_n^{\overline{\text{MS}}}(n_\ell - 1, 1) \left(\frac{\alpha_s^{(n_\ell)}(\bar{m}_q)}{4\pi} \right)^n = m_Q^{\text{pole}} - \bar{m}_q, \end{aligned} \quad (3.21)$$

where we have used the $\xi = 1$ constraint. For the MSRp scheme HQS is not exact, but the correction is calculable in perturbation theory and thanks to the $\xi = 1$ constraint happens to be identical to the MSRn to $\overline{\text{MS}}$ matching condition:

$$m_Q^{\text{pole}} - m_Q^{\text{MSRp}}(\bar{m}_q) - [m_Q^{\text{pole}} - \bar{m}_q] = \text{HQS}(\bar{m}_q, n_\ell - 1, 2). \quad (3.22)$$

Therefore HQS corrections can be calculated even if the lighter quark finite mass effects have not been computed yet, as long as the massless corrections are known. The R-anomalous dimension is modified as a consequence of the finite lighter quark mass:

$$\begin{aligned} -\frac{d}{dR} m_Q^{\text{MSR}}(R) &= \gamma^R[\alpha_s^{(n_\ell)}(R)] + \delta\gamma^R[\xi_R, \alpha_s^{(n_\ell)}(R)], \\ \delta\gamma^R[\xi_R, \alpha_s^{(n_\ell)}(R)] &= \sum_{n=1} \delta\gamma_n^R(\xi_R) \left(\frac{\alpha_s^{(n_\ell)}(R)}{4\pi} \right)^{n+1}, \\ \delta\gamma_n^R(\xi_R) &= \Delta_n(\xi_R) - \xi_R \frac{d\Delta_n(\xi_R)}{d\xi_R} - 2 \sum_{j=0}^{n-2} (n-j) \beta_j \Delta_{n-j}(\xi_R). \end{aligned} \quad (3.23)$$

This equation can be integrated either numerically as it stands, or recast into a form that factors out Λ_{QCD} , as explained in ref. [60]. Given that the $\mathcal{O}(\alpha_s^4)$ finite lighter quark mass corrections are unknown, we will cut the sum of the second term strictly at $n = 3$, even if there are lower order Δ terms that contribute at $n = 4$ in the sum over j . Such decision

¹⁰In ref. [42] the MSR mass with light massive quarks was implemented differently: $\delta m_Q^{\text{MSR}}(R, \bar{m}_q) = \delta m_Q^{\text{MSR}}(R) + \bar{m}_q \Delta_{\bar{m}_q}(\bar{m}_Q, \bar{m}_q/\bar{m}_Q)$, which is well suited to study the large-order behavior of the series. With this definition the R-evolution equation is the same as for massless lighter quarks, but one might have potentially large logs of the form $\log(R/\bar{m}_Q)$ when implementing the MSR scheme in a perturbative series. With this definition one needs to include Heavy Quark Symmetry breaking corrections to the MSRn mass when integrating out the massive lighter quark, whereas with our implementation these corrections are absent.

Figure 2. Finite lighter quark mass corrections to the R-anomalous dimension at two and three loops. The various pieces in which $\delta\gamma_2^R$ (left panel) and $\delta\gamma_3^R$ (right panel) are decomposed are shown separately. These pieces correspond to the terms shown in eq. (3.23).

is adopted because the inclusion of such terms could overestimate the real size of that correction if large cancellations happen. These cancellations are indeed expected since Δ_n are afflicted by a renormalon but $\delta\gamma_R^n$ are not. In figure 2 this is graphically depicted at two and three loops, where it is seen that the effect is larger at smaller ξ . Since the cancellations are expected to be larger for high values of n (where the renormalon dominates), we can estimate $\Delta_4(r)$ by requiring that $\delta\gamma_3^R(\xi) = 0$. In general one would have:

$$\Delta_n(\xi) \approx \xi \Delta_n(1) + 2\xi \sum_{j=0}^{n-2} (n-j) \beta_j \int_{\xi}^1 dx \frac{\Delta_{n-j}(x)}{x^2}, \quad (3.24)$$

where $\Delta_n(1)$ are known from the $\xi = 1$ constraint. Eq. (3.24) automatically satisfies the $\xi = 1$ and $\xi = 0$ constraints. If this approximation is used from $n = 1$ one gets the following predictions:

$$\begin{aligned} \Delta_2(\xi)^{\text{app}} &= \xi \Delta_2(1), \\ \Delta_3(\xi)^{\text{app}} &= \xi \Delta_3(1) - 4\beta_0 \Delta_2(1) \xi \log(\xi), \\ \Delta_4(\xi)^{\text{app}} &= \xi \Delta_4(1) - [4\beta_1 \Delta_2(1) + 6\beta_0 \Delta_r(1)] \xi \log(\xi) + 12\beta_0^2 \Delta_2(1) \xi \log^2(\xi). \end{aligned} \quad (3.25)$$

This approximation corresponds to the estimate made in eqs. (3.12) and (3.13) of ref. [42] if one sets $\mu = \overline{m}_Q$ [see eq. (3.14) of that reference]. Since Δ_2 and Δ_3 are exactly known, we can use them to make a better prediction for Δ_4 , which we call Δ_4^{best} . To test this method, one can also use the known expression of Δ_2 to predict Δ_3 , calling it again Δ_3^{best} , and consider the difference of Δ_3^{best} and Δ_3^{app} as an estimate of the uncertainty of this procedure. We observe that Δ_3^{best} is a better approximation to Δ_3 than Δ_3^{app} , and that Δ_3 is contained in the uncertainty band, although quite close to its upper bound. This is depicted in figure 3a. Finally one can compute the estimate of Δ_4 which uses the exact form of Δ_2 and Δ_3^{best} , which we call Δ_4^{good} . We observe that Δ_4^{good} is closer to Δ_4^{best} than

Figure 3. (a) Estimate of the three-loop massive lighter quark effects on the relation between the $\overline{\text{MS}}$ and pole masses for $n_\ell = 4$ (blue band) versus the exact result (red line). (b) Estimate of the four-loop term Δ_4 for $n_\ell = 4$ (upper red band) and $n_\ell = 5$ (lower blue band). The uncertainty bands are estimated from the difference of two consecutive orders of the approximation. (c) Lighter massive quark correction to the $\mathcal{O}(\alpha_s^2)$ term of the $\overline{\text{MS}}$ -pole relation. In red the exact form of eq. (3.17) is shown, while blue shows the linear approximation of eq. (3.24).

Δ_4^{app} . The difference between Δ_4^{good} and Δ_4^{best} will be used to estimate the uncertainty on Δ_4^{best} , which happens to be 2% at worst across the whole spectrum for either 4 or 5 light flavors. Our estimate is shown graphically in figure 3b. Our prediction for Δ_4 and its uncertainty band can be parametrized with the following fit functions:

$$\begin{aligned} \Delta_4(n_\ell = 4) &= \xi [120472 + 35\xi + (2201\xi + 20909)\log^2(\xi) + (-3768\xi - 76707)\log(\xi)] \\ &\quad \pm \xi [5\xi + (-2667\xi - 375)\log^2(\xi) + (5459\xi - 5430)\log(\xi)], \\ \Delta_4(n_\ell = 5) &= \xi [102238 + 33\xi + (1966\xi + 17620)\log^2(\xi) - (3011\xi + 66608)\log(\xi)] \\ &\quad \pm \xi [7\xi - (2208\xi + 388)\log^2(\xi) + (4873\xi - 4811)\log(\xi)]. \end{aligned} \quad (3.26)$$

The method of requiring a vanishing R-anomalous dimension is not as powerful in predicting the massless coefficients, and for those one needs to know at least the one-loop term. For instance, for $n_\ell = 4$, and assuming that all orders lower than the one that is predicted are known, one gets:

$$\begin{aligned} a_2^{\overline{\text{MS}}}(n_\ell = 4, 0) &= 89[130], & a_3^{\overline{\text{MS}}}(n_\ell = 4, 0) &= 5400 \pm 1900, \\ a_4^{\overline{\text{MS}}}(n_\ell = 4, 0) &= 330000 \pm 36000, & a_5^{\overline{\text{MS}}}(n_\ell = 4, 0) &= (232 \pm 7) \times 10^5, \end{aligned} \quad (3.27)$$

there the quoted uncertainty corresponds to the difference of the central value and the prediction that assumes that the previous order is also estimated with this method. The exact results for $a_n^{\overline{\text{MS}}}(n_\ell = 4, 0)$ for $n = 2, 3, 4$ are 130.128, 4582.54, 214100.

Finally, we note that the uncertainty associated to the absence of the Δ_4 , $\delta\gamma_3^R$ and $\delta E_X^{(3)}$ terms can be estimated by comparing the schemes with n_ℓ and $(n_\ell - 1)$ dynamical flavors.

3.4 MSR mass in the n_ℓ flavor scheme

The MSR mass described in section 3.3 accounts for the charm mass corrections explicitly, as it considers the charm quark a dynamical flavor. However there are physical situations

in which, due to the energy scales involved, it is convenient to integrate out the charm quark as well. For bottomonium, the charm mass is sufficiently large compared to the non-relativistic scales to assume one is close to the decoupling limit, i.e., $\bar{m}_c \rightarrow \infty$. Indeed, the closeness of the exact finite-charm mass corrections of section 2.2 to the decoupling limit for scales around 1 to 4 GeV points to such conclusion. In that case, the charm quark can be integrated out and one should switch to an $(n_\ell - 1)$ -flavor MSR scheme with the charm quark decoupled to all orders in Υ expansion, reducing to a theory with $(n_\ell - 1)$ dynamical flavors.

We define the MSR mass with n_ℓ active flavors, either Natural or Practical, as follows:

$$m_Q^{\text{pole}} - m_Q^{\text{MSR}(n_\ell-1)}(R) = m_q^{\text{pole}} - m_q^{\text{MSR}}(R), \quad (3.28)$$

where it is understood that m_q^{MSR} has $(n_\ell - 1)$ dynamical flavors. Therefore, the R-evolution in this scheme does not include charm mass effects, and its relation to the pole mass has only $(n_\ell - 1)$ flavors. One needs to connect the $m_Q^{\text{MSR}(n_\ell-1)}$ mass to $\bar{m}_Q$, and if large logs of $\bar{m}_Q/\bar{m}_q$ are to be avoided, one should not directly subtract eqs. (3.28) and (3.16). R-evolution can sum up these logs if the relation is organized as follows:

$$\begin{aligned} m_Q^{\text{MSR}(n_\ell-1)}(R) &= \left[m_Q^{\text{MSR}(n_\ell-1)}(R) - m_Q^{\text{MSR}(n_\ell-1)}(\bar{m}_q) \right] + \left[m_Q^{\text{MSR}(n_\ell-1)}(\bar{m}_q) - m_Q^{\text{pole}} \right] \\ &\quad + \left[m_Q^{\text{pole}} - m_Q^{\text{MSR}'(\bar{m}_q)} \right] + \left[m_Q^{\text{MSR}'(\bar{m}_q)} - m_Q^{\text{MSR}'(\bar{m}_Q)} \right] + \left[m_q^{\text{MSR}'(\bar{m}_Q)} - \bar{m}_Q \right] + \bar{m}_Q \\ &= \left[m_q^{\text{MSR}}(R) - m_q^{\text{MSR}}(\bar{m}_q) \right] + \left[m_q^{\text{MSR}}(\bar{m}_q) - \bar{m}_q \right] + \left[\bar{m}_q - m_q^{\text{pole}} \right] + \left[m_Q^{\text{pole}} - m_Q^{\text{MSR}'(\bar{m}_q)} \right] \\ &\quad + \left[m_Q^{\text{MSR}'(\bar{m}_q)} - m_Q^{\text{MSR}'(\bar{m}_Q)} \right] + \left[m_Q^{\text{MSR}'(\bar{m}_Q)} - \bar{m}_Q \right] + \bar{m}_Q, \end{aligned} \quad (3.29)$$

where one can use different versions of the MSR mass in the n_ℓ and $(n_\ell - 1)$ schemes, hence we distinguish them with a prime. We have used eq. (3.28) in the first and second terms in square brackets of the first line to get to the second line. One uses R-evolution to sum up logs of $R/\bar{m}_q$ and $\bar{m}_q/\bar{m}_Q$ in the first and fifth terms in square brackets, respectively. The second and one-to-last terms in square brackets are the $\overline{\text{MS}}$ -MSR matching conditions, which are zero in the Practical scheme. The sum of the third and fourth terms in square brackets correspond to the HQS breaking expression, which is zero in the Natural scheme. In practice one can write eq. (3.29) as

$$m_Q^{\text{MSR}(n_\ell-1)}(R) = m_q^{\text{MSR}}(R) - \bar{m}_q + \text{HQS}'(\bar{m}_q, n_\ell - 1, 2) + m_Q^{\text{MSR}'(\bar{m}_q)}, \quad (3.30)$$

where m_q^{MSR} and $m_Q^{\text{MSR}'}$ include matching to the $\overline{\text{MS}}$ mass and R-evolution, and $\text{HQS} = 0$ if MSR' is the Natural scheme. The sequence of R-running and matching can be better visualized in figure 4.

In ref. [41] the finite charm quark mass corrections to a three-flavor bottom quark $\overline{\text{MS}}$ mass are computed in fixed-order, without R-evolution. In our notation that computation corresponds to $\bar{m}_b - m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_b)$. One could decompose this difference into various

Figure 4. Graphical representation of the sequence of R-running and matching that one needs to carry out to evaluate the $\text{MSR}^{(n_\ell)}$ and $\text{MSR}^{(n_\ell-1)}$ masses.

pieces that sum up logarithms

$$\begin{aligned}
 & \bar{m}_b - m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_b) \\
 &= \left[m_b^{\text{MSRp}}(\bar{m}_b) - m_b^{\text{MSRp}}(\bar{m}_c) \right] + \left[m_b^{\text{MSRp}}(\bar{m}_c) - m_b^{\text{pole}} \right] \\
 & \quad + \left[m_b^{\text{pole}} - m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_c) \right] + \left[m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_c) - m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_b) \right] \\
 &= \left[m_b^{\text{MSRp}}(\bar{m}_b) - m_b^{\text{MSRp}}(\bar{m}_c) \right] + \text{HQS}(\bar{m}_c) + \left[m_c^{\text{MSRp}}(\bar{m}_c) - m_c^{\text{MSRp}}(\bar{m}_b) \right],
 \end{aligned} \tag{3.31}$$

where we have used that $\bar{m}_b = m_b^{\text{MSRp}}(\bar{m}_b)$. The first and last terms in brackets sum up logarithms of $\bar{m}_b/\bar{m}_c$. Since these are not very large, we find that our result is not in contradiction with ref. [41]. Taking $\bar{m}_b = 4.2 \text{ GeV}$, $\bar{m}_c = 1.3 \text{ GeV}$, $\alpha_s^{(n_f=5)}(m_Z) = 0.1181$ we find $\bar{m}_b - m_b^{\text{MSRp}(n_\ell-1)}(\bar{m}_b) = 0.05 \pm 0.05 \text{ GeV}$, where the error comes from scale variation in the R-evolution.¹¹

4 Scale variation and charm quark mass effects

In this section we perform a numerical investigation of the scale variation that one needs to perform to properly estimate uncertainties coming from missing uncalculated higher-order terms.¹² These unknown terms appear in the perturbative expansion for the quarkonium energy levels as well as on the relation between the pole and $\overline{\text{MS}}$ masses. The way one estimates the former is varying the scale μ , while varying R provides an estimate for the latter. The range in which these two parameters should be varied depends on the principal

¹¹Ref. [50] computes the similar quantity $\bar{m}_b - m_b^{\text{MSRn}(n_\ell-1)}(\bar{m}_b)$, finding an effect which is also compatible with zero. We find $0.04 \pm 0.04 \text{ GeV}$, using our slightly different MSR definition. Furthermore, in our uncertainty estimate of HQS we probe scales a factor of two smaller (larger) than their lowest (highest) scale.

¹²For the numerics in this article we run α_s with the five-loop beta function, and we match at the various quark mass thresholds taking the five-loop expression with $\mu_q = \bar{m}_q$. For the MSR mass we perform 4-loop massless R-evolution (and matching to $\bar{m}_q$) and include finite charm mass corrections at three loops. The matching between the $\text{MSR}^{(n_\ell=4)}$ and $\text{MSR}^{(n_\ell=3)}$ masses is performed at four loops.

quantum number n . For μ this is easy to see, since n appears in the argument of the perturbative logarithms. Since there are logarithms of μ/R in the MSR mass subtractions, R has to be of the same order of μ , and that is how the R variation inherits its n dependence. In any case we observe that changing the value of R in a given range causes variations on the predicted masses much smaller than varying μ in the same range. Therefore we interpret that μ variation estimates the error coming from missing higher order terms in the theoretical expression for the bound-state masses, whereas R variation accounts for the arbitrariness that one has in connecting the relativistic $R \sim \bar{m}_Q$ and non-relativistic regimes $R \sim \bar{m}_Q \alpha_s C_F$, in the same way that one uses the MSR mass to smoothly match the 1S mass into the $\overline{\text{MS}}$ one. For simplicity we use the same range of variation for both μ and R .

We will start with the usual procedure to figure out the “natural” value of the renormalization scale: μ_{nat} has to be such that the argument of the perturbative logarithms equals unity. To estimate the range of variation we can simply require that the argument of the logarithms becomes $2^{\pm\phi}$: $(\mu_{\text{nat}} \pm \Delta\mu) \sim 2^{\pm\phi} C_F \alpha_s^{(n_\ell)}(\mu) m_Q/n$, where the specific value of m_Q depends on the scheme one is using, and one can adjust the value of ϕ or even take different values for upwards or downwards variations. For this numerical exercise we take $m_Q = m_Q^{\text{MSR}}(R = \mu)$ and half of the average of the masses of states with principal quantum number n (experimental values). Both choices yield similar results: for bottomonium and taking $\phi = 0.5$ we find for $n = 1, 2$ the following ranges: $\mu_{n=1} \sim 1.9_{-0.4}^{+1.6} \text{ GeV}$, $\mu_{n=2} \sim 1.25 \pm 0.25 \text{ GeV}$. Most of the variation from this ranges comes from the lower edge, therefore we simplify the scale variations to $1.5 \text{ GeV} \geq \mu_{n=1} \geq 4 \text{ GeV}$ and $1 \text{ GeV} \geq \mu_{n=2} \geq 4 \text{ GeV}$. We observe that using these ranges the estimated uncertainty bars make the results compatible order by order in perturbation theory, as can be seen in figures 5a and 5b. We observe that for $n = 1$ a turnover takes place between N²LO and N³LO, as the error bar increases when increasing the order of perturbation theory, contrary to the expectations. We observe that this behavior persists even if the lower scale in the variation range is reduced to 1 GeV. For $n = 2$ this does not happen and the minimal uncertainty is achieved at the highest perturbative order, as expected. It is hard to pin down the origin of this behavior, but one could imagine that some sort of accidental numerical cancellation happens at N²LO and $n = 1$, which makes the renormalization scale variation method underestimate the actual uncertainty due to missing higher order terms. This behavior is obviously transmitted to the extraction of the heavy quark masses.

The same exercise for $n = 3$ yields a lower bound below 1 GeV, presumably too low for perturbation theory to work. Therefore we try the same variations as for $n = 1, 2$, and as shown in figures 5b and 5c none of these choices is satisfactory: the $n = 1$ variation makes the N³LO prediction incompatible with the LO and NLO results; on the other hand the $n = 2$ variation makes the error bars equally large for all orders. We therefore conclude that perturbation theory is not applicable for values of n equal or larger than 3.

The same analysis for charmonium again yields values for the natural scale μ below 1 GeV. In this case we take a completely heuristic approach and choose the scale variation such that there is order-by-order convergence and agreement. We find that varying the scales in the range $1.2 \text{ GeV} \geq \mu_{\text{charm}} \geq 4 \text{ GeV}$ gives a pattern very similar to the $n = 1$ bottomonium states, as can be seen by comparing figures 5a and 7a.

Figure 5. Prediction for the bottomonium masses up to $n = 3$ for various perturbative orders. The top figures show the two $n = 1$ states with a scale variation of μ and R between 1.5 GeV and 4 GeV (left plot) and $n = 2$ with variation between 1 GeV and 4 GeV (right plot). The two lower plots have the same scale variation as the corresponding upper plots, but both show results for $n = 3$.

Finally let us compare our considerations for natural renormalization scales with the so called Principle of Minimal Sensitivity (PMS for short). For this exercise we consider the MSRp scheme with $R = \overline{m}_Q$. This mimics the $\overline{\text{MS}}$ scheme for charmonium and for bottomonium in the $\alpha_s^{(n_\ell=4)}$ scheme. For bottomonium in the $\alpha_s^{(n_\ell=3)}$ scheme it is similar to the $\overline{\text{MS}}$ scheme, but with R-evolution summing up logarithms of $\overline{m}_c/\overline{m}_b$. We make this choice because it is the most similar to what is used in refs. [30, 54], while the outcome of this analysis in the MSRn scheme is very similar. Our results are shown in figure 6. We find that the PMS largely depends on the perturbative order one is considering: only in the two highest orders a maximum is attained, and between these two differences as large as 3 GeV for $n = 1$ bottomonium states occur, and around 1 GeV in the other cases we studied. There is a moderate dependence on the number of flavors one is using (1 GeV at worst). In the case of bottom, the highest order $\overline{\text{MS}}$ scheme with $n_\ell = 3$ shows both a minimum and a maximum for the ground state. For $n = 1$ the maximum position is biased towards large (relativistic) scales.

Figure 6. Canonical scales according to the principle of minimal sensitivity. The left (a), center (b) and right (c) panels show the bottomonium $\Upsilon(1^3S_1)$ and $\Upsilon(2^3S_1)$ states, and the charmonium $J/\psi(1S)$ state, respectively. In (a) and (b) the solid line shows the $\alpha_s^{(n_\ell=4)}$ scheme, whereas dashed lines correspond to the $\alpha_s^{(n_\ell=3)}$ scheme. Green, blue, purple and red colors represent LO, NLO, N^2 LO and N^3 LO predictions, respectively. Whenever a maximum is attained, its position is marked with a fat colored dot.

The last thing we want to explore in this section is the m_c dependence of the bottomonium binding energies and the various ways in which the charm quark mass corrections can be implemented. As discussed already in section 2.2, one can assume a massless charm quark to which one adds non-zero charm quark mass corrections [what we call the $\alpha_s^{(n_\ell=4)}$ scheme], or one can assume a theory with a decoupled (that is, integrated out) charm quark to which one adds corrections to the decoupling limit [what we call the $\alpha_s^{(n_\ell=3)}$ scheme]. In refs. [30, 41] it has been argued that the latter is the most accurate description, because the decoupling limit is much closer to the physical situation than the massless limit. Here we confirm this claim, and actually show that it holds for almost any value of the charm quark mass, as can be seen in figure 7b: the decoupling limit and the $\alpha_s^{(n_\ell=3)}$ scheme are much close to one another than the massless limit and the $\alpha_s^{(n_\ell=4)}$ scheme for most values of the charm mass, except for very small values of m_c where (as expected) the two former blow up. The main reason for the proximity of the decoupling limit and the $\alpha_s^{(n_\ell=3)}$ scheme is that for both of them the dependence on the charm quark mass comes mainly from $\alpha_s^{(n_\ell=3)}$ and $m_b^{\text{MSR}(n_\ell=3)}$, whereas the massless limit has no dependence on $\overline{m}_c$ at all, while the $\alpha_s^{(n_\ell=4)}$ scheme depends on the charm quark mass through corrections to the static energy and the $\overline{\text{MS}}$ pole dependence.

5 Fits to experimental data

We have created two independent computer codes, one (slow) written in Mathematica [61] and another one (fast) written in Fortran 2008 [62]. Both codes agree within 8 significant digits. The duplication of the code allows a cross-check of all the formulas and procedures described above, giving confidence in our results. For our numerical analysis we mainly use the Fortran code.

The aim of our code is to compute the perturbative mass of a heavy quarkonium state with arbitrary quantum numbers [eq. (2.1)] in the MSR mass scheme¹³ as a function of the

¹³Our code can also be run in the pole and $\overline{\text{MS}}$ schemes.

Figure 7. Left panel: mass of the $n = 1$ charmonium states at various perturbative orders. Blue and red colors correspond to the masses of the J/Ψ and η_c particles, respectively. The error bars correspond to a scale variation between 1.2 GeV and 4 GeV. Right panel: mass of the $\Upsilon(1^3S_1)$ bottomonium bound state in the MSRn scheme as a function of the charm mass in the $\overline{\text{MS}}$ scheme. The blue and red lines show the $\alpha_s^{(n_f=4)}$ and $\alpha_s^{(n_f=3)}$ schemes, respectively. The green line corresponds to the $\alpha_s^{(n_f=3)}$ scheme with no further finite charm mass corrections implemented. The horizontal gray dashed line shows the $\bar{m}_c = 0$ approximation in the $\alpha_s^{(n_f=4)}$ scheme, while the vertical dashed gray line signals the world average value for the charm quark mass.

$\overline{\text{MS}}$ mass of the heavy quark and two renormalization scales μ and R . For a given dataset, the value of $\bar{m}_Q$ is extracted from the minimum of the following χ^2 function, which depends on a set of pairs of renormalization scales $\{\mu_n, R_n\}$, one for each principal quantum number that appears in the dataset:

$$\chi^2(\{\mu_n, R_n\}) = \sum_i \left(\frac{M_i^{\text{exp}} - M_i^{\text{pert}}(\mu_i, R_i, \bar{m}_Q)}{\sigma_i^{\text{exp}}} \right)^2, \quad (5.1)$$

where the sum extends to the individual states in the given dataset and M_i^{exp} and σ_i^{exp} are the experimental masses and errors extracted from the PDG [63]. Such fit would give us a best-fit $\overline{\text{MS}}$ mass value as a function of μ_n and R_n .

One could think the optimal way of including theoretical uncertainties in our fits is by adding these as part of the χ^2 functions. The problem is that theoretical errors are highly correlated among various states, as stems from the following facts:

1. All masses are determined from the same static potential. Therefore whatever the unknown N⁴LO static potential is, it is the same for all states. Varying the renormalization scale μ uncertainties coming from this and higher-order unknown terms are estimated. Therefore the value of μ has to be varied in a correlated way for all states included in the dataset.
2. All masses in a short-distance scheme use the same $\overline{\text{MS}}$ -pole mass relation to cancel the factorially divergent behavior, and no matter how the $\mathcal{O}(\alpha_s^5)$ correction looks like,

it is going to be the same for all states. Uncertainties coming from this and higher order uncalculated terms are estimated varying the scale R . Therefore the value of R has to be varied in a correlated way for all states in the dataset.

3. All masses depend on the same value of $\alpha_s^{(n_f=5)}(m_Z)$ and $\overline{m}_c$, therefore uncertainties associated to these two quantities are obviously 100% correlated.

We performed a numerical study to estimate the theoretical error matrix and found the correlation is very close to 100%. Given that perturbative errors greatly dominate over experimental uncertainties, a fit including such a highly correlated error matrix is severely affected by the so-called d’Agostini bias [64], resulting in a global best-fit value which is considerably lower than individual determinations from each state in the dataset. Two possible ways out of this problem are: a) perform global fits with χ^2 functions which depend on μ and R ; b) determine the heavy quark masses from fits to individual states and a posteriori perform a weighted average of the best-fit results. For the latter one has to compute the weighted average using only the experimental errors, since the highly correlated theoretical errors cannot judge the quality of individual results (and would again cause the bias towards small values). The theoretical uncertainty is then estimated as the average of the individual theoretical uncertainties. In a more formal way, this is achieved by using for the weighted average a theoretical correlation matrix in which each entry is substituted by the average of all the entries in the original matrix. This procedure is quite standard, and it is motivated by the idea that the parameter one is fitting for is unique, and therefore its theoretical error is unique as well, being the average of its various estimates the least biased approximation. A theoretical error matrix exactly proportional to the unit matrix avoids the d’Agostini bias and yields as the result of the fit precisely the weighted average with experimental uncertainties only. For our analysis we take approach a) as our default and use b) as a validation of our results. We find both methods are in quite good agreement, although in some cases b) yields slightly larger perturbative uncertainties.

In order to estimate the dependence of $\overline{m}_Q$ with the renormalization scales we vary them, within reasonable ranges, in an independent way. The specific energy windows for each scale depend on the convergence behavior for each heavy quarkonium state. As already argued in section 4, for $n = 1$ states one should vary the renormalization scales between $(\mu_1, R_1) \in [1.5, 4] \text{ GeV}$, whereas for states with $n = 2$ one should rather take the ranges $(\mu_2, R_2) \in [1, 4] \text{ GeV}$. For $n = 3$ states perturbation theory is already badly behaved such that scales around 1 GeV are too low and the perturbative series starts to fail, which significantly increases the error associated to the scales. For that reason, the ranges used for $n = 3$ will be $(\mu_3, R_3) \in [1.5, 4] \text{ GeV}$, which still yields uncertainty bars much larger than for $n = 1, 2$ states. In any case $n = 3$ states are only used as an illustration and do not enter our final numbers. Since the μ_n and R_n scales have to be varied together to account for theory correlations we use the following parametrization: $\mu_2(\mu) = \mu$, $R_2(R) = R$, $\mu_{1,3}(\mu) = 1.5 \text{ GeV} + 2.5 (\mu - 1 \text{ GeV})/3$, $R_{1,3}(R) = 1.5 \text{ GeV} + 2.5 (R - 1 \text{ GeV})/3$, and vary μ and R between 1 GeV and 4 GeV. This linear rescaling for $n = 1, 3$ implements the correct correlation to the $n = 2$ state avoiding unnaturally low scales, and makes the χ^2 function dependent on the global μ and R only. The central value for $\overline{m}_Q$ will be calculated as the average of all the best-fits on a (μ, R) grid.

From the χ^2 minimization we extract the uncertainty coming from the experimental error of the heavy quarkonium masses, denoted as Δ^{exp} . Around the best-fit value of a given (μ, R) pair, the χ^2 function can be approximated by

$$\chi^2 \approx \chi_{\text{min}}^2 + \left(\frac{\bar{m}_Q - \bar{m}_Q^{\text{BF}}}{\Delta^{\text{exp}}} \right)^2. \quad (5.2)$$

The central value for the experimental error will be taken as the average of all the Δ^{exp} in the (μ, R) grid (which happen to be all very similar). Due to the high accuracy of the PDG heavy quarkonium masses up to $n = 3$, such uncertainty is very small.

The largest source of uncertainty will be that associated to the variation of the scales, dubbed Δ^{pert} . Its value will be taken as the difference of the maximum and minimum best-fit values in the grid:

$$\Delta^{\text{pert}} = \frac{1}{2} \left[\max(\bar{m}_Q^{\text{BF}}(\mu, R)) - \min(\bar{m}_Q^{\text{BF}}(\mu, R)) \right]. \quad (5.3)$$

Finally, the errors associated to the uncertainty on the strong coupling Δ^{α_s} (using the 2016 PDG world average $\alpha_s^{(n_f=5)}(m_Z) = 0.1181 \pm 0.0011$ [63]) and, for the bottom mass fits, the charm mass $\Delta^{\bar{m}_c}$ ($\bar{m}_c = 1.28 \pm 0.03 \text{ GeV}$ [63]) will be computed by repeating the fits using the $1\text{-}\sigma$ upper and lower values for these quantities, and taking the half of the differences of the respective resulting best-fit values.¹⁴

For our fits we have followed two complementary methods, which we have carried out independently as an extra check. In our first strategy we created grids in $\bar{m}_Q$ for the theoretical prediction of each individual state. We created different grids for each pair $\{\mu, R\}$ in the grid and theoretical setup. The grids are then combined into χ^2 functions for the various datasets, which are minimized to fit for the bottom mass. The second strategy computes the bottom mass from individual states numerically solving the equation $M_{\text{theo}} = M_{\text{exp}}$. We find that this equation can be solved iteratively to arbitrary precision, and that with 10 iterations one obtains 10 significant digits. In order to perform global fits to multiple states, in this second strategy we directly minimize the χ^2 function numerically using the COMPASS_SEARCH [65] routine. Both methods agree in more than three significant digits.

5.1 Bottomonium fits and determination of $\bar{m}_b$

In this section we present the core result of our analysis, the determination of the bottom quark mass. We provide results for fits to 14 individual bottomonium states (all states with $n \leq 3$), as well as for global fits, for which we create a few datasets:

1. $\text{Set}_{n=1} = \{ \eta_b(1S), \Upsilon(1S) \}.$
2. $\text{Set}_{n=2} = \{ \chi_{b0}(1P), \chi_{b1}(1P), h_b(1P), \chi_{b2}(1P), \eta_b(2S), \Upsilon(2S) \}.$
3. $\text{Set}_{n=3} = \{ \Upsilon(1D), \chi_{b0}(2P), \chi_{b1}(2P), h_b(2P), \chi_{b2}(2P), \Upsilon(3S) \}.$

¹⁴For charmonium fits we proceed in the same way with the bottom quark mass PDG value to determine the associate error $\Delta^{\bar{m}_b}$.

4. $\text{Set}_{L=P} = \{ \chi_{b0}(1P), \chi_{b1}(1P), h_b(1P), \chi_{b2}(1P) \}$.
5. $\text{Set}_{n \leq 2} = \text{Set}_{n=1} \cup \text{Set}_{n=2}$.
6. $\text{Set}_{n \leq 3} = \text{Set}_{n=1} \cup \text{Set}_{n=2} \cup \text{Set}_{n=3}$.

Our results at $N^3\text{LO}$ are collected in tables 1 and 2 for the MSRn and MSRp schemes, respectively, and in figure 8a for the MSRn scheme with $n_\ell = 3$ active flavors. The table presents the results using perturbative expansions in terms of $\alpha_s^{(n_\ell=4)}$ and $\alpha_s^{(n_\ell=3)}$, shown in the left and right blocks, respectively. In columns second to fifth we split the error in its various contributions: experimental, perturbative, and due to the uncertainties in $\alpha_s^{(n_f=5)}(m_Z)$ and $\bar{m}_c(\bar{m}_c)$. We observe that the perturbative uncertainty clearly dominates over the rest, followed by the $\alpha_s^{(n_f=5)}(m_Z)$ error. The error due to the uncertainty on the charm mass is negligible. The experimental uncertainty deserves a more detailed explanation: for individual fits it is negligibly small in all cases, but for global fits we modify it to account for the large values of the $\chi_{\min}^2$. For instance, in the $\text{Set}_{n \leq 2}$ we get $\chi_{\min}^2/\text{d.o.f.} = 21300$, indicating that the theoretical accuracy is much less than the experimental precision. In order to correct for this deficiency of our fits, we inflate our experimental fit uncertainties by a factor such that $\chi_{\min}^2/\text{d.o.f.}$ becomes unity. This procedure cannot be applied to individual fits as for those both $\chi_{\min}^2$ and d.o.f are identically zero. Lower orders for $\text{Set}_{n=1}$, $\text{Set}_{n=2}$ and $\text{Set}_{n \leq 2}$ in the MSRn scheme with $n_\ell = 3$ active flavors are shown in figure 8b. Finally in figure 9a we show the results of various global fits at $N^3\text{LO}$ in the MSRn scheme both with $n_\ell = 4$ and $n_\ell = 3$ active flavors.

Following the observations made in ref. [41], which we confirmed in section 4, we favor the expansion with $n_\ell = 3$ flavors over $n_\ell = 4$, and take it for our final determination. In any case, the perturbative uncertainties are slightly larger for $n_\ell = 3$ [see figure 9a], so our choice is conservative. Furthermore, we consider $\text{Set}_{n \leq 2}$ as our default, as all states contained in it can be accurately described within perturbation theory, and is less biased than taking only ground states. Finally, we observe that the difference between the MSRn and MSRp schemes is at the sub-MeV level for the central values, (0.02%) but the MSRn scheme yields perturbative uncertainties 13 MeV (28%) smaller than the MSRp. Accordingly we consider the MSRn scheme (which is also theoretically cleaner) as our default, finding our final result for the bottom mass:

$$\begin{aligned} \bar{m}_b(\bar{m}_b) &= 4.216 \pm 0.009_{\text{exp}} \pm 0.034_{\text{pert}} \pm 0.017_{\alpha_s} \pm 0.0008_{\bar{m}_c} \text{ GeV} \\ &= 4.216 \pm 0.039 \text{ GeV} . \end{aligned} \quad (5.4)$$

If one uses a correlated scale variation setting $\mu = R$ the central value decreases by 1 MeV and the perturbative error shrinks to 18 MeV. If we set $R = 4 \text{ GeV}$ the result reads $\bar{m}_b = 4.233 \pm 0.010_{\text{pert}} \pm \dots$ with a central value 17 MeV larger and perturbative error roughly a factor of 3 smaller. We have performed fits with $\bar{m}_c = 0$ and in the decoupling limit. The former is 30 MeV above the result in eq. (5.4) while the latter is 4.7 MeV below. The result in the $n_\ell = 4$ scheme is 8.6 MeV higher than our final result with $n_\ell = 3$. If we add this difference to our uncertainties to account for effects of missing higher-order charm mass corrections we would get a total error of 40 MeV. If we add the difference between

States	$\alpha_s^{(n_\ell=4)}$					$\alpha_s^{(n_\ell=3)}$				
	$\overline{m}_b$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_c}$	$\overline{m}_b$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_c}$
$\eta_b(1S)$	4.219	0.0011	0.045	0.005	0.0004	4.210	0.0011	0.046	0.006	0.0001
$\Upsilon(1S)$	4.234	0.0001	0.048	0.005	0.0004	4.226	0.0001	0.048	0.007	0.0002
$\chi_{b0}(1P)$	4.195	0.0002	0.039	0.020	0.0006	4.187	0.0002	0.050	0.020	0.0010
$\chi_{b1}(1P)$	4.207	0.0002	0.036	0.020	0.0006	4.200	0.0002	0.046	0.021	0.0010
$h_b(1P)$	4.209	0.0004	0.036	0.021	0.0006	4.201	0.0004	0.045	0.021	0.0010
$\chi_{b2}(1P)$	4.214	0.0002	0.035	0.021	0.0006	4.206	0.0002	0.044	0.021	0.0010
$\eta_b(2S)$	4.233	0.0018	0.044	0.023	0.0006	4.222	0.0018	0.065	0.023	0.0012
$\Upsilon(2S)$	4.241	0.0001	0.040	0.023	0.0006	4.230	0.0001	0.059	0.024	0.0012
$\Upsilon(1D)$	4.244	0.0006	0.057	0.027	0.0006	4.238	0.0006	0.072	0.028	0.0014
$\chi_{b0}(2P)$	4.265	0.0003	0.063	0.029	0.0006	4.257	0.0003	0.080	0.029	0.0015
$\chi_{b1}(2P)$	4.274	0.0002	0.064	0.029	0.0006	4.267	0.0002	0.081	0.029	0.0015
$h_b(2P)$	4.276	0.0005	0.064	0.029	0.0006	4.269	0.0005	0.081	0.029	0.0015
$\chi_{b2}(2P)$	4.280	0.0002	0.064	0.029	0.0006	4.272	0.0002	0.081	0.029	0.0015
$\Upsilon(3S)$	4.309	0.0002	0.070	0.030	0.0006	4.301	0.0002	0.088	0.030	0.0016
$n = 1$	4.234	0.0017	0.048	0.005	0.0004	4.225	0.0018	0.048	0.007	0.0002
$n = 2$	4.219	0.0081	0.033	0.021	0.0006	4.210	0.0078	0.042	0.022	0.0011
$n = 3$	4.282	0.0080	0.065	0.029	0.0006	4.275	0.0079	0.083	0.029	0.0015
$L = P$	4.207	0.0039	0.036	0.020	0.0006	4.199	0.0039	0.046	0.021	0.0010
$n \leq 2$	4.225	0.0084	0.030	0.016	0.0005	4.216	0.0089	0.034	0.017	0.0008
$n \leq 3$	4.240	0.0100	0.021	0.019	0.0005	4.231	0.0106	0.032	0.020	0.0010

Table 1. Results for $\overline{m}_b$ fits for different set of states in the MSRn scheme at N³LO. The first 14 rows correspond to fits to individual states, whereas the last 6 rows show global fit results. Columns 2 to 6 and 7 to 11 show the $\alpha_s^{(n_\ell=4)}$ and $\alpha_s^{(n_\ell=3)}$ schemes, respectively. Within each flavor-scheme block, the uncertainty is split in columns second to fifth into experimental, perturbative, due to uncertainty in $\alpha_s^{(n_f=5)}(m_Z)$ and due to uncertainty in $\overline{m}_c(\overline{m}_c)$, respectively. For the various global fits the error associated to the experimental uncertainty (that is, the error coming from the fit) is rescaled by the factor $\sqrt{\chi^2_{\text{min}}/\text{d.o.f.}}$. All masses and errors are expressed in GeV.

Set _{$n=1$} and Set _{$n=2$} as an estimate of non-perturbative effects our total uncertainty would raise to 43 MeV (44 MeV if both effects are considered simultaneously). At the sight of this, we believe our uncertainty of 39 MeV is conservative enough.

In figure 9b and table 3 the predictions for $n \leq 3$ bottomonium masses are shown at N³LO using our best-fit value for the bottom quark mass. From the results it is evident that the experimental precision is far superior than the theoretical accuracy. Finally we explore the dependence of our final result on the value of $\alpha_s^{(n_f=5)}(m_Z)$, finding

$$\begin{aligned} \overline{m}_b(\overline{m}_b) = & 4.216 - 14.587(\alpha_s - 0.1181) \pm 0.0005_{\text{exp}} \pm 0.0008_{\overline{m}_c} \\ & \pm [0.0341332 + 7.91281(\alpha_s - 0.1181) + 798.251(\alpha_s - 0.1181)^2]_{\text{pert}} \text{ GeV}. \end{aligned} \quad (5.5)$$

The central value rapidly decreases as $\alpha_s^{(n_f=5)}(m_Z)$ grows, but the perturbative error mildly increases [see figure 10a].

States	$\alpha_s^{(n_\ell=4)}$					$\alpha_s^{(n_\ell=3)}$				
	$\overline{m}_b$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_c}$	$\overline{m}_b$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_c}$
$\eta_b(1S)$	4.219	0.0011	0.047	0.005	0.0004	4.210	0.0011	0.048	0.006	0.0001
$\Upsilon(1S)$	4.234	0.0001	0.050	0.005	0.0004	4.226	0.0001	0.050	0.007	0.0002
$\chi_{b0}(1P)$	4.196	0.0002	0.054	0.020	0.0006	4.189	0.0002	0.069	0.020	0.0010
$\chi_{b1}(1P)$	4.208	0.0002	0.052	0.020	0.0006	4.201	0.0002	0.066	0.021	0.0010
$h_b(1P)$	4.210	0.0004	0.051	0.020	0.0006	4.203	0.0004	0.065	0.021	0.0010
$\chi_{b2}(1P)$	4.215	0.0002	0.050	0.020	0.0006	4.207	0.0002	0.063	0.021	0.0010
$\eta_b(2S)$	4.234	0.0018	0.049	0.022	0.0006	4.223	0.0018	0.066	0.023	0.0012
$\Upsilon(2S)$	4.242	0.0001	0.046	0.023	0.0006	4.232	0.0001	0.060	0.023	0.0012
$\Upsilon(1D)$	4.244	0.0006	0.057	0.027	0.0006	4.238	0.0006	0.072	0.028	0.0014
$\chi_{b0}(2P)$	4.265	0.0003	0.064	0.028	0.0006	4.257	0.0003	0.081	0.029	0.0015
$\chi_{b1}(2P)$	4.274	0.0002	0.064	0.029	0.0006	4.267	0.0002	0.081	0.029	0.0015
$h_b(2P)$	4.276	0.0005	0.065	0.029	0.0006	4.269	0.0005	0.082	0.029	0.0015
$\chi_{b2}(2P)$	4.280	0.0002	0.065	0.029	0.0006	4.273	0.0002	0.082	0.029	0.0015
$\Upsilon(3S)$	4.309	0.0002	0.070	0.030	0.0006	4.301	0.0002	0.089	0.030	0.0016
$n = 1$	4.234	0.0017	0.050	0.005	0.0004	4.226	0.0018	0.050	0.007	0.0002
$n = 2$	4.220	0.0081	0.048	0.021	0.0006	4.212	0.0078	0.060	0.022	0.0011
$n = 3$	4.282	0.0080	0.066	0.029	0.0006	4.275	0.0079	0.083	0.029	0.0015
$L = P$	4.208	0.0039	0.052	0.020	0.0006	4.201	0.0039	0.065	0.021	0.0010
$n \leq 2$	4.225	0.0083	0.041	0.016	0.0005	4.217	0.0088	0.048	0.016	0.0008
$n \leq 3$	4.240	0.0100	0.029	0.019	0.0005	4.232	0.0105	0.034	0.020	0.0010

Table 2. Same as table 1 for the MSRp scheme.

5.2 Charmonium fits and determination of $\overline{m}_c$

One can use the master formula in eq. (2.6) in the MSR scheme to compute the masses of $c\bar{c}$ bound states. One simplification with respect to bottomonium is that there are no lighter quarks with mass larger than Λ_{QCD} , therefore there are no corrections from finite masses of lighter quarks. On the other hand the physical scales in the problem are smaller, hence one expects much larger perturbative (as well as non-perturbative) uncertainties. As discussed in section 4, we will restrict our analysis to $n = 1$ states and will vary μ and R between 1.2 GeV and 4 GeV, which yields order-by-order convergence and agreement with moderate perturbative uncertainties. We will perform individual (state by state) and global ($n = 1$) fits, which are summarized at N³LO in table 4, whereas lower orders are shown graphically in figure 11a. We find that the result of the global fit is almost identical to the individual fit to the J/ψ state. This is nothing but expected given that the experimental uncertainty of J/ψ is 80 times smaller than that of η_c . However, the combined fit yields very large χ^2_{min} values, of the order of 45700, indicating that the theory accuracy is much worse than the experimental one. Therefore we apply the same rescaling procedure already applied in the bottom fits.

Figure 8. 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 N³LO in the MSRn scheme with $n_\ell = 3$ active flavors. Right panel: global fits to $n = 1$ (blue), $n = 2$ (green) and $n = 1, 2$ (red) as a function of the perturbative order NⁿLO. The PDG world average value is shown with a gray band. Both panels: only perturbative uncertainties shown.

Figure 9. Left panel: bottom quark mass determined at N³LO in the MSRn scheme with $n_\ell = 4$ (blue) and $n_\ell = 3$ (red) flavors from global fits to $n = 1$, $n = 2$, $n = 3$, $n = 1, 2$ and $n = 1, 2, 3$ states. Right panel: prediction of the bottomonium energy levels at N³LO (in blue) vs the corresponding experimental values (in red). Experimental error bars are too small to be visible.

Our results are collected in table 4 for the MSRn (left block) and MSRp (right) schemes. The error is divided into various contributions: experimental, perturbative, and due to the uncertainties in α_s and $\bar{m}_b(\bar{m}_b)$. For the latter we take the 2016 world average $\bar{m}_b = 4.18^{+0.04}_{-0.03} \text{ GeV}$ [63]. Same as we did for the bottom analysis, we observe that theoretical uncertainties greatly dominate over α_s uncertainties, and again experimental uncertainties (coming from the fit procedure) are negligibly small. The $\bar{m}_b$ uncertainty is, as expected, tiny, as the dependence on the bottom mass comes only from the α_s thresh-

Figure 10. Dependence of the bottom (left panel) and charm (right panel) quark masses on the value of $\alpha_s^{(n_f=5)}(m_Z)$. The determinations correspond to global fits for the $n = 1, 2$ (bottom) and $n = 1$ (charm) states. The MSRn scheme is used at N³LO order, in both cases in terms of $\alpha_s^{(n_f=3)}$.

State	n	$2s+1\ell_j$	M_{exp} [GeV]	$M_{\text{pert}}^{(n_\ell=3)}$ [GeV]
$\eta_b(1S)$	1	1S_0	9.3990(23)	9.41 ± 0.10
$\Upsilon(1S)$	1	3S_1	9.46030(26)	9.44 ± 0.10
$\chi_{b0}(1P)$	2	3P_0	9.85944(52)	9.92 ± 0.11
$\chi_{b1}(1P)$	2	3P_1	9.89278(40)	9.93 ± 0.10
$h_b(1P)$	2	1P_1	9.8993(8)	9.93 ± 0.10
$\chi_{b2}(1P)$	2	3P_2	9.91221(40)	9.93 ± 0.09
$\eta_b(2S)$	2	1S_0	9.999(4)	9.99 ± 0.14
$\Upsilon(2S)$	2	3S_1	10.02326(31)	9.99 ± 0.13
$\Upsilon(1D)$	3	3D_2	10.1637(14)	10.12 ± 0.16
$\chi_{b0}(2P)$	3	3P_0	10.2325(6)	10.14 ± 0.18
$\chi_{b1}(2P)$	3	3P_1	10.25546(55)	10.14 ± 0.18
$h_b(2P)$	3	1P_1	10.2598(12)	10.14 ± 0.18
$\chi_{b2}(2P)$	3	3P_2	10.26865(55)	10.14 ± 0.18
$\Upsilon(3S)$	3	3S_1	10.3552(5)	10.17 ± 0.20

Table 3. Masses of the bottomonium states, up to $n = 3$, calculated with the perturbative formula of eq. (2.1) and with $n_\ell = 3$ dynamical flavors. The results are computed with the final bottom quark fit value of $\bar{m}_b = 4.216$ GeV.

old matching from 5 to 4 flavors. Within three-digit rounding, the total and perturbative errors are the same.

We observe that the difference between the MSRn and MSRp schemes is 1 MeV for the central values, (0.4%) but the MSRn scheme yields perturbative uncertainties 9 MeV (10%) smaller than the MSRp. Accordingly we again consider the MSRn scheme as our default, and taking the global fit as the least biased we find our final result for the charm mass:

$$\begin{aligned}\overline{m}_c(\overline{m}_c) &= 1.273 \pm 0.0005_{\text{exp}} \pm 0.054_{\text{pert}} \pm 0.006_{\alpha_s} \pm 0.0001_{\overline{m}_b} \text{ GeV} \\ &= 1.273 \pm 0.054 \text{ GeV},\end{aligned}\tag{5.6}$$

where we have symmetrized the error due to the uncertainty of $\overline{m}_b$. If one uses a correlated scale variation setting $\mu = R$ the central value does not change within three digits but the perturbative error shrinks to 40 MeV. If we set $R = \overline{m}_c$ the result reads $\overline{m}_c = 1.310 \pm 0.009_{\text{pert}} \pm \dots$. If we change the Υ -scheme counting to the non-relativistic counting (see discussion in section 6) the central value becomes 20 MeV smaller. Similarly, if we employ the iterative method of eq. (2.8) the central value grows 20 MeV. These variations are much larger than what we find in the bottom analysis, reflecting that perturbation theory is obviously less convergent for charmonium. Nevertheless they are well contained in our estimate for higher-order corrections. Finally, if we add the difference between the results to individual fits to J/ψ and η_c to our error budget to estimate non-perturbative corrections, our combined uncertainty would increase to 68 MeV.

In figure 11b and table 5 we show the prediction for $n = 1$ charmonium states at N³LO using eq. (5.6) for charm quark mass. It appears very clear that the experimental precision is far superior than the theoretical accuracy. We also explore the dependence of the central value and perturbative error with $\alpha_s^{(n_f=5)}(m_Z)$. We again find a rather linear dependence of the former while the latter is best approximated by a quadratic fit form:

$$\begin{aligned}\overline{m}_c(\overline{m}_c) &= 1.273 - 5.793 (\alpha_s - 0.1181) \pm 0.0005_{\text{exp}} \pm 0.0001_{\overline{m}_b} \\ &\quad \pm [0.054 + 12.66 (\alpha_s - 0.1181) + 1219.11 (\alpha_s - 0.1181)^2]_{\text{pert}} \text{ GeV}.\end{aligned}\tag{5.7}$$

The situation is the opposite as for the bottom mass: the central value slowly decreases as $\alpha_s^{(n_f=5)}(m_Z)$ grows, but the perturbative error rapidly increases [see figure 10b].

5.3 Simultaneous fits to $\overline{m}_b$ and $\alpha_s^{(n_f=5)}(m_Z)$

The large value of χ^2 per degree of freedom in fits to the bottomonium spectrum and the big amount of precise data at our disposal suggests that one could fit another parameter. In this section we briefly elaborate on the possibility of performing a simultaneous fit to both the bottom quark mass and the strong coupling constant, as was first suggested in ref. [30]. The first observation is that, for fixed values of the renormalization scales, one only breaks the degeneracy between α_s and $\overline{m}_b$ if states with principal quantum number $n = 1$ and $n = 2$ are included. For our default dataset $n \leq 2$ and fixed values of the renormalization scales we can determine both parameters with great precision: $4.5 \times 10^{-3} \%$ for the bottom mass and $9.7 \times 10^{-3} \%$ for α_s . The experimental correlation between these is $\rho = -0.92$ in average.

States	MSRn					MSRp				
	$\overline{m}_c$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_b}$	$\overline{m}_c$	Δ^{exp}	Δ^{pert}	Δ^{α_s}	$\Delta^{\overline{m}_b}$
η_c	1.232	2×10^{-4}	0.070	0.005	$+7 \times 10^{-5}$ -9×10^{-5}	1.233	2×10^{-4}	0.078	0.005	$+6 \times 10^{-5}$ -8×10^{-5}
J/ψ	1.273	2.7×10^{-6}	0.054	0.006	$+8 \times 10^{-5}$ -11×10^{-5}	1.274	2.7×10^{-6}	0.063	0.006	$+8 \times 10^{-5}$ -11×10^{-5}
$n = 1$	1.273	5×10^{-4}	0.054	0.006	$+8 \times 10^{-5}$ -11×10^{-5}	1.274	5×10^{-4}	0.063	0.006	$+8 \times 10^{-5}$ -11×10^{-5}

Table 4. Results for $\overline{m}_c$ fits for different set of states at N³LO. The error is split by their different contributions. All masses and errors are expressed in GeV. Columns 2 to 5 and 6 to 9 show the MSRn and MSRp schemes, respectively. Within each scheme block, the uncertainty is split in columns second to fifth into experimental, perturbative and due to uncertainty in $\alpha_s^{(n_f=5)}(m_Z)$ and $\overline{m}_b$, respectively. For the $n = 1$ fits the error associated to the experimental uncertainty (that is, the error coming from the fit) is rescaled by the factor $\sqrt{\chi_{\min}^2}$.

State	n	$^{2s+1}\ell_j$	M_{exp} [GeV]	M_{pert} [GeV]
$\eta_c(1S)$	1	1S_0	2.9834(5)	3.07 ± 0.14
$J/\psi(1S)$	1	3S_1	3.096900(6)	3.10 ± 0.10

Table 5. Masses of the charmonium states with $n = 1$, calculated with the perturbative formula of eq. (2.1). The results are computed with the final charm quark fit value of $\overline{m}_c = 1.273$ GeV.

This nice scenario deteriorates once we perform scale variation in the ranges explained in section 5, yielding sizable perturbative uncertainties and correlating both parameters even more ($\rho = -0.99$). The average $\chi^2/\text{d.o.f.}$ decreases by a factor of 2.6 from 21300 to 8045. We find

$$\begin{aligned} \overline{m}_b(\overline{m}_b) &= 4.219 \pm 0.0002_{\text{exp}} \pm 0.062_{\text{pert}} \text{ GeV}, \\ \alpha_s^{(n_f=5)}(m_Z) &= 0.1178 \pm 0.00001_{\text{exp}} \pm 0.0050_{\text{pert}}. \end{aligned} \quad (5.8)$$

Rescaling the experimental errors by $\sqrt{\chi^2/\text{d.o.f.}}$ the uncertainties increase to 0.016 GeV and 0.0010 for $\overline{m}_b$ and α_s , respectively. Although the uncertainty on α_s is only 4% (good in absolute terms), and our determination is certainly compatible with the world average, it cannot compete with its current precision, which is at the percent level.

6 Comparison with previous determinations

We finish our analysis by comparing our results with recent previous determinations, either using quarkonium energy levels or other observables. We split our comparison in bottom and charm analyses.

Bottom quark mass. In figure 12a we compare our result for the bottom quark mass with other determinations that also use bottomonium energy levels. We compare to the N²LO analysis of ref. [30] and the N³LO analyses of refs. [53, 54]. While our analysis and those of refs. [30, 53] use the $n_\ell = 3$ flavor scheme as the reference calculation, ref. [54] uses

Figure 11. Left panel: charm quark mass determination from the η_c (blue), J/ψ (green) and both states together (red) as a function of the perturbative order NⁿLO. The PDG world average value is shown with a gray band. Right panel: prediction of the charmonium masses at N³LO (in blue) vs the corresponding experimental values (in red). Experimental error bars are too small to be visible. Both panels: predictions in the MSRn scheme where the error bars correspond to the perturbative uncertainties only.

$n_\ell = 4$ for the main analyses and takes the $n_\ell = 3$ computation to estimate uncertainties due to the finite charm quark mass. While refs. [30, 53] fit only to the $\Upsilon(1S)$ state and ref. [54] considers both states with $n = 1$, we include all states with principal quantum number $n \leq 2$. Ref. [54] takes for their final determination the (unweighted) average of the individual determinations for $\Upsilon(1S)$ and $\eta_b(1S)$, while we perform global fits which take into account theoretical correlations and weight each individual state by its experimental uncertainty. Refs. [30] and [54] use the $\overline{\text{MS}}$ scheme and vary scales according to the principle of minimal sensitivity. Finally, ref. [30] uses $\alpha_s^{(n_f=5)}(m_Z) = 0.1181 \pm 0.0020$, [53] $\alpha_s^{(n_f=5)}(m_Z) = 0.1184 \pm 0.0007$, and [54] $\alpha_s^{(n_f=5)}(m_Z) = 0.1185 \pm 0.0007$.

Our theoretical treatment is very similar to that of ref. [53], since both analyses use a low-scale short-distance mass (MSR vs RS). As for scale variation, for $n = 1$ it is identical for μ , while the lower limit for R is 1 GeV in ref. [53], as opposed to our 1.5 GeV. On the other hand we vary both scales independently on a square grid, while ref. [53] varies one scale at a time. Both our central values and theoretical uncertainties are in excellent agreement.

The theoretical error found in ref. [54] is only 20 MeV, half the size of ours, while their central value is 19 MeV lower. This uncertainty estimate is based on the PMS, for which the canonical scales are found to be 5.352 GeV and 6.157 GeV for the $\Upsilon(1S)$ and $\eta_b(1S)$ states, respectively. We already argued in section 4 those values are unnaturally large for a non-relativistic system of bottom quarks. The uncertainty is then estimated by comparing the results of the canonical scale with those that use twice that scale. Since the variation is only towards larger scales, the variance found is rather small: 21 MeV and 18 MeV, respectively. We also observe that this scale variation leads to a slight inconsistency between LO and N³LO results.

Figure 12. Comparison of our determination of the bottom $\overline{\text{MS}}$ mass (in red) with previous results from bottomonium (left) and other methods (right). Panel (a) compares a result at N²LO (second from the bottom in blue), with three results at N³LO. In these analyses various schemes for the bottom mass and different scale variations are used. Panel (b) shows the outcome of our analysis, a lattice determination (blue), two results from non-relativistic sum rules (purple) and one from relativistic sum rules (green). Both panels: the PDG world average value is shown as a vertical gray band. Note that the PDG world average has asymmetric uncertainties.

The result of ref. [30] is 26 MeV lower than ours, but still in full agreement. But being only an N²LO analysis, it claims an uncertainty due to missing higher order corrections of 25 MeV, which is 26% smaller than our estimate. This analysis also uses the PMS to fix the scale, but the perturbative uncertainty is obtained by estimating the effect of different implementations of the Υ -expansion scheme. In our code we can also use two counting schemes, depending how one considers the scaling of the parameter R . The Υ -expansion scheme considers $R \sim m_Q$, but in the so called non-relativistic counting one takes $R \sim m_Q \alpha_s$. The difference between our results in the Υ -scheme and non-relativistic counting is 6 MeV. We can also compare our results with the expanded out and iterative methods of eqs. (2.7) and (2.8),¹⁵ finding differences below 6 MeV. All these are much smaller than our perturbative uncertainty.

In figure 12b we compare the outcome of our analysis with determinations of the bottom mass from other observables. We compare to a Lattice determination [66], one relativistic [67] and two non-relativistic [58, 68] sum rule analyses.¹⁶ Ref. [66] uses a non-relativistic lattice action to compute high moments of the vector correlator.¹⁷ These are compared to relativistic continuum perturbation theory to extract the bottom quark mass,

¹⁵These equations can be recast into an expression for the binding energy of the state, and can therefore be implemented into our χ^2 function.

¹⁶The result of ref. [58] has been updated in [69] with the four-loop coefficient of the $\overline{\text{MS}}$ -pole mass relation.

¹⁷Another recent lattice determination can be found in ref. [70], which computes the ratio m_b/m_c on the lattice and determines m_b from their m_c lattice determination. They obtain $\bar{m}_b = 4.184 \pm 0.089$ GeV. The same approach was used in ref. [71] which found $\bar{m}_b = 4.162 \pm 0.048$ GeV. These results are less precise than the direct determination of [66] $\bar{m}_b = 4.196 \pm 0.023$ GeV.

Figure 13. Comparison of various charm quark mass determinations from charmonium fits [red (this work) and purple], relativistic QCD sum rules (green) and Lattice QCD (blue). The PDG world average value is shown as a vertical gray band.

a procedure that could be called into question. Refs. [58, 68] use non-relativistic sum rules in a low-scale short-distance scheme, but the former uses fixed-order perturbation theory at N³LO while the latter performs large-log resummation at (partial) N²LL in the framework of vNRQCD. Finally ref. [67] uses the second moment of the vector correlator in the $\overline{\text{MS}}$ scheme and varies independently the scales associated to α_s and $\overline{m}_b$. The error from relativistic sum rules are generically smaller since low-energy scales are not being probed.

Charm quark mass. In figure 13 we compare our charm quark mass determination with a selection of previous results, which include relativistic sum rules [67], Lattice QCD [71] and fits to the lowest lying charmonium states [54]. In the following we discuss the latter by itself, and two former together.

Let us start by comparing our result in eq. (5.6) with the analysis of ref. [54], which also uses non-relativistic QCD at N³LO, but employing the $\overline{\text{MS}}$ short-distance scheme. Furthermore, the principle of minimal sensitivity is used to set the default renormalization scale μ , finding 2.14 GeV and 2.42 GeV for J/ψ and η_c , respectively. These are much larger than what we find from requiring a small size for the perturbative logarithms (~ 1 GeV). Finally, the perturbative uncertainty is estimated by setting the renormalization scale to twice the minimal sensitivity value. That yields for the average of their individual determinations an uncertainty of 23 MeV, which is a factor of two smaller than our estimate. Their central value is 27 MeV smaller than ours, but results are compatible within errors. Finally, while we perform a global fit to both $n = 1$ states, which takes into account theoretical correlations, ref. [54] determines the charm mass from J/ψ and η_c individually and computes the (unweighted) average of those as their final determination.

The analyses of refs. [67, 71] use relativistic sum rules at $\mathcal{O}(\alpha_s^3)$ for the vector and pseudo-scalar correlators, respectively.¹⁸ Although the analyses look similar at first glance, they differ in the way perturbative uncertainties are estimated. While [67] varies renormal-

¹⁸A similar lattice analysis can be found in ref. [70] with the result $\overline{m}_c = 1.267 \pm 0.012$ GeV, which is less precise than the value obtained in [71], $\overline{m}_c = 1.2715 \pm 0.0095$ GeV.

ization scales associated to α_s and $\overline{m}_c$ independently in the range $\overline{m}_c$ to 4 GeV, ref. [71] sets $\mu = 3$ GeV and makes an educated guess for missing higher order corrections, resulting in a much smaller perturbative error. The investigations performed in ref. [67] suggest that the convergence of the pseudo-scalar perturbative series is significantly worse than of the vector correlator, and that the theoretical uncertainty of ref. [71] might be underestimated. The reader is referred to ref. [67] for more details on the analysis.

7 Conclusions

In this work we have studied the bottomonium and charmonium spectra within Non-Relativistic QCD at the perturbative level up to N³LO. For the former we have considered corrections coming from the finite charm quark mass up to N²LO, and studied setups with $n_\ell = 3$ and $n_\ell = 4$, concluding that the former is very close to the decoupling limit and likely captures most of the finite charm quark mass effects. To cancel the $\mathcal{O}(\Lambda_{\text{QCD}})$ renormalon of the QCD static potential we employ the low-scale short distance MSR mass, realized in its Practical and Natural versions. We make a dedicated study of scale setting by requiring that the perturbative logarithms become minimal, and choose to vary around that canonical scale such that the size of the argument of those logarithms departs 40% from unity. We vary the renormalization scale μ and the infrared scale R independently in the same range. With this prescription we find that bottomonium states with principal quantum number n smaller than 3 can be described within perturbation theory, but for $n = 3$ states no convergence is found. For charmonium we find that $n = 1$ states can be predicted although the convergence of perturbation theory is significantly worse. One could argue that a more appropriate short-distance mass for bottomonium physics is, for instance, the 1S mass [38–40], which does not explicitly depend on any additional low-energy scale.¹⁹ However R variation accounts for the uncertainty associated in the conversion of the 1S mass into the $\overline{\text{MS}}$ mass, in which the MSR mass plays the role of a smooth interpolator between typical non-relativistic scales of the order of the inverse of the Bohr radius and relativistic scales as the mass itself.

For bottomonium we include effects of the charm quark mass in the R-evolution of the MSR mass, what ensures there are no Heavy Quark Symmetry breaking corrections for the Natural MSR mass. Furthermore, requiring that the massive R-anomalous dimension vanishes we predict the uncalculated $\mathcal{O}(\alpha_s^4)$ virtual massive quark corrections to the relation between the $\overline{\text{MS}}$ and pole masses, and obtain an (iterative) expression for these corrections in the asymptotic limit. We also define the MSR scheme with $(n_\ell - 1)$ flavors, which is smoothly connected to the $\text{MSR}^{(n_\ell)}$ scheme at the scale $R = \overline{m}_q$. Of course the $\text{MSR}^{(n_\ell)}$ scheme is also smoothly connected to the $\overline{\text{MS}}$ scheme at $R = \overline{m}_Q$, what makes our connection between the $\text{MSR}^{(n_\ell-1)}$ and $\overline{\text{MS}}$ schemes smooth. In this context smooth means summing up large logarithms of ratios of scales.

¹⁹Other equally suitable masses include the PS mass [28], which we have discarded due to its dependence on a factorization scale at $\mathcal{O}(\varepsilon^4)$, the RS [34], Kinetic [35] and jet [36, 37] masses, which we discard because either they are not known to the required accuracy or do not include finite charm quark mass effects.

To determine the bottom and charm quark masses we compare to individual states and perform global fits. Since theoretical uncertainties are highly correlated among the various states we perform fits for given values of the renormalization scales, and scan over those in a grid to determine the uncertainties due to missing higher-order corrections. Since the lowest bound in which these scales are varied depends on the principal quantum number, we correlated the values of μ and R for each value of n by rescaling the $n = 1$ scales to the appropriate ranges. For our final result we choose the most complete dataset that includes states with $n \leq 2$ for bottom and $n = 1$ for charm. Taking the MSR $_n$ scheme with $n_\ell = 3$ active flavors in both cases we find:

$$\begin{aligned}\bar{m}_b(\bar{m}_b) &= 4.216 \pm 0.039 \text{ GeV} , \\ \bar{m}_c(\bar{m}_c) &= 1.273 \pm 0.054 \text{ GeV} ,\end{aligned}\tag{7.1}$$

where all errors have been added in quadrature, but are fairly dominated by the perturbative uncertainties. We have compared our results with previous determinations which use either quarkonium spectroscopy or other methods, and find good agreement with all of them and with the world average. Our estimate of the uncertainty due to missing higher-order corrections is larger than those of refs. [30, 54], which use the principle of minimal sensitivity, but very similar to that of ref. [53], which varies both μ and R scales independently (but one at a time) in a range similar to ours.

We have also explored the possibility of performing simultaneous fits to $\bar{m}_b$ and α_s , finding that if both $n = 1$ and 2 states are included a fit to both parameters is possible. We find:

$$\begin{aligned}\bar{m}_b(\bar{m}_b) &= 4.219 \pm 0.064 \text{ GeV} , \\ \alpha_s^{(n_f=5)}(m_Z) &= 0.1178 \pm 0.0051 ,\end{aligned}\tag{7.2}$$

where again all errors have been added in quadrature and are completely dominated by theoretical uncertainties. The bottom quark mass uncertainty grows by 64%, and the uncertainty on α_s , although good in absolute terms, cannot compete with recent determinations that reach $\sim 1\%$.

Let us close this article discussing possible improvements on our analysis. Although the study performed in this article suggests that non-perturbative effects are small for $n = 1$ and 2, a more systematic study of these could make our phenomenological observation into a definite statement. Having higher-order corrections in the near future seems unrealistic, but one could perform the analysis using a renormalization-group-improved theoretical expression, possibly in the context of pNRQCD. This would sum up ultra-soft effects that already arise at $\mathcal{O}(\varepsilon^4)$, deteriorating the convergence of the perturbative series. One would expect that such an RGE analysis would yield smaller perturbative uncertainties, from which the charmonium analysis would particularly benefit. On the other hand, one could incorporate the whole QCD static potential at the leading-order Hamiltonian and carry out perturbation theory around it, as in the study of ref. [72]. Finally one could use our estimate for the $\mathcal{O}(\alpha_s^4)$ charm mass correction to the $\overline{\text{MS}}$ -pole mass relation and the decoupling limit approximation to estimate the missing finite charm quark mass corrections at $\mathcal{O}(\varepsilon^4)$, and check if this brings the $n_\ell = 3$ and $n_\ell = 4$ schemes closer to each another.

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A Formulas

In this appendix we provide some expressions related to the finite charm quark mass correction. In the definition of the $\mathcal{O}(\varepsilon^2)$ correction to the binding energy $\delta E_X^{(1)}$ we need the expression for the function $f_D(n, \ell, k, x)$, which can be written as

$$f_D(n, \ell, k, x) = \frac{d^{2n-1}}{dx^{2n-1}} \left[(2 - x^4 - x^2) x^{2k+2\ell+1} \begin{pmatrix} \frac{\cos^{-1}(\frac{1}{x})}{\sqrt{x^2-1}} & x > 1 \\ 1 & x = 1 \\ \frac{\log\left(\frac{\sqrt{1-x^2}+1}{x}\right)}{\sqrt{1-x^2}} & x < 1 \end{pmatrix} \right], \quad (\text{A.1})$$

where $\rho = (2n m_c^{\text{pole}})/[R C_F \alpha_s^{(4)}(\mu)]$. Furthermore, the $\mathcal{O}(\varepsilon^3)$ charm-mass correction to the binding energy $\delta E_X^{(2)}$ in the decoupling limit ($m_c \rightarrow \infty$) is

$$\begin{aligned} (\delta E_X^{(2)})_{m_c \rightarrow \infty} = & - \left(\frac{\alpha_s^{(4)}(\mu)}{4\pi} \right)^2 \frac{4C_F^2 \alpha_s^{(4)}(\mu)^2 m_b^{\text{pole}}}{n^2} \left\{ \log\left(\frac{\mu}{m_c^{\text{pole}}}\right) \left(\frac{13}{18} - c_1^{(n_\ell-1)} - \frac{2n_\ell}{9} \right) \right. \\ & + L_n \left[\left(\frac{35}{2} - n_\ell \right) c_1^{(n_\ell-1)} + \left(n_\ell - \frac{33}{2} \right) c_1^{(n_\ell)} + \frac{2n_\ell - 35}{3} \log\left(\frac{\mu}{m_c^{\text{pole}}}\right) \right. \\ & \left. \left. + \frac{8n_\ell - 79}{18} \right] + \frac{1}{3} \log^2\left(\frac{\mu}{m_c^{\text{pole}}}\right) - \frac{2}{3} (n_\ell - 17) L_n^2 - \frac{7}{12} + c_2^{(n_\ell-1)} - c_2^{(n_\ell)} \right\}, \\ L_n = & \log\left(\frac{n\mu}{C_F \alpha_s^{(4)}(\mu) m_b^{\text{pole}}}\right) + H_{\ell+n}. \end{aligned} \quad (\text{A.2})$$

Finally, the three-loop correction from massive lighter quarks to the relation between the pole and the $\overline{\text{MS}}$ masses, $\Delta_3^{(g, n_\ell, n_h)}$ is parametrized with a Padé approximants, as detailed in section 3.2. The terms of eq. (3.18) have the following form:

$$\begin{aligned} \Delta_3^{(g)}(\xi) = & \frac{\xi}{\xi + 6.5849} \left[121.713\xi^8 + 43.0875\xi^7 + 75.8986\xi^6 - 40.2407\xi^5 \right. \\ & + 1143.85\xi^4 + 2861.3\xi^3 + (26.0741\xi + 171.695)\xi^3 \log^3(\xi) + 4621.34\xi^2 \\ & + \xi^3 \log^2(\xi) (-19.545\xi^5 - 128.702\xi^4 - 54.5284\xi^3 - 359.064\xi^2 - 81.4937\xi) \\ & - 536.628 + (-6.2695\xi^8 - 76.1755\xi^7 - 194.437\xi^6 + 50.0976\xi^5 - 1217.64\xi^4 \\ & - 1300.47\xi^3 - 8551.79\xi^2 - 5659.48\xi - 7609.65) \log(\xi) - 4387.21\xi \\ & \left. + 9379.48 \right] + \frac{8}{3} \Delta_2^{\overline{\text{MS}}}(\xi), \end{aligned} \quad (\text{A.3})$$

$$\Delta_3^{(n_\ell)}(\xi) = \frac{\xi}{\xi+1.46064} \left[0.430408\xi^8 - 0.657671\xi^7 + 5.88658\xi^6 - 14.0718\xi^5 - 69.2551\xi^4 \right. \\ \left. - 18.3617\xi^3 + (-4.74074\xi - 6.9245)\xi^3 \log^3(\xi) + (15.4074\xi + 22.5046)\xi^3 \log^2(\xi) \right. \\ \left. + 36.737\xi^2 + (-0.161088\xi^8 - 0.235292\xi^7 - 1.70667\xi^6 - 2.49282\xi^5 + 18.0613\xi^4 \right. \\ \left. + 96.5648\xi^3 + 102.513\xi^2 + 70.1839\xi + 102.513) \log(\xi) - 45.6933\xi - 97.084 \right],$$

$$\Delta_3^{(n_h)}(\xi) = \frac{\xi^2}{\xi-1.47336} \left[0.13153\xi^7 - 0.123376\xi^6 + 3.92059\xi^5 - 5.77644\xi^4 + 7.36885\xi^3 \right. \\ \left. - 29.5727\xi^2 + (0.457144\xi^3 - 0.673537\xi^2 + 1.8963\xi - 2.79393)\xi^4 \log^2(\xi) \right. \\ \left. + (-0.0772789\xi^7 + 0.11386\xi^6 - 3.60296\xi^5 + 5.30846\xi^4 - 11.1477\xi^3 \right. \\ \left. + 16.4246\xi^2 + 0.0000225622\xi - 0.0000332423) \log(\xi) + 41.7971\xi - 20.9544 \right],$$

where $\xi = \overline{m}_c/\overline{m}_b$.

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