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Quarkonium Spectroscopy and Perturbative QCD : A New Perspective

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Abstract

We study the energy spectrum of bottomonium in perturbative QCD, taking $\alpha_{\rm s}(M_Z) = 0.1181 \pm 0.0020$ as input and fixing $m_b^{\overline{\rm MS}}(m_b^{\overline{\rm MS}})$ on the $\Upsilon(1S)$ mass. Contrary to wide beliefs, perturbative QCD reproduces reasonably well the gross structure of the spectrum as long as the coupling constant remains smaller than one. We perform a detailed analysis and discuss the size of non-perturbative effects. A new qualitative picture on the structure of the bottomonium spectrum is provided. The lowest-lying $c\bar{c}$ and $b\bar{c}$ states are also examined.

1 Introduction

In recent years our knowledge of heavy quarkonia in the framework of perturbative QCD has developed significantly. On one hand computations of new higher-order corrections to various physical quantities appeared [1, 2, 3, 4]. On the other hand the discovery of the mechanism of the renormalon cancellation in the quarkonium spectrum [5, 6] led to a drastic improvement of the convergence of the perturbative expansion of the energy levels. As important applications up to date, the theory enabled precise determinations of the $\overline{\rm MS}$-mass of the bottom quark [7, 8, 9, 10] and (in the future) of the top quark [11] from (mainly) the energy spectra of the lowest-lying states. The main uncertainty comes, in the bottomonium case, from the (essentially) unknown non-perturbative contributions. These are generally claimed to be around 100 MeV and ultimately set the precision of the prediction.

As for the structure of the higher quarkonium levels, the Coulomb potential seems to be unable to explain it (for a review see [12]). For instance, the spacing between two consecutive nS levels does not decrease with n and appears roughly constant. For this reason several confining potentials have been introduced in the literature over the last decades. We refer to [13] for one of the most recent phenomenological study on several of them. Progress in this direction seems to be no longer possible, as far as the relation of the confining potentials with QCD remains obscure. This relation has been elucidated recently in [14, 15] where a complete and systematic parametrization inside QCD of perturbative and non-perturbative effects of the heavy quarkonium interaction has been realized. The parametrization depends on the mutual relation between the scale of non-perturbative physics, $\Lambda_{\rm QCD}$, and the other dynamical scales in the specific heavy quarkonium system under study. A way to determine it and the size and nature of the non-perturbative contributions, consists in establishing to which extent perturbative QCD can consistently and successfully describe the system. This is the aim of the present paper, which investigates the range of validity of perturbative QCD on the heavy quarkonium spectroscopy and consequently extracts upper bounds to the non-perturbative contributions by comparing the perturbative predictions, at the current best accuracy, with the experimental data.

One of the main problems in having a consistent (i.e. convergent) perturbative expansion for the quarkonium energy levels has been for a long time its bad behaviour when expressed in terms of the pole mass (see, for instance, the poor convergence of the computations reported in [16, 7]). The reason has been understood in the renormalon language: the pole mass [17] and the QCD static potential [18], respectively, contain renormalon contributions of order $\Lambda_{\rm QCD}$, which get cancelled in the total energy of a color singlet quark-antiquark system [5, 6]. The solution then consists in making explicit this cancellation by substituting in the energy expansion a short-range mass (free from infrared ambiguities) for the pole mass. In [10, 9, 4] this approach has been used in order to calculate the bottom quark mass by means of sum rules. However, an analysis of the consistency between the whole level structure of perturbative QCD and the experimental data is lacking and will be done in the present work. In order to make explicit the renormalon cancellation we will express the quarkonium energies in terms of the $\overline{\rm MS}$ masses and rearrange the perturbative series in the so-called ε expansion [19]. This will be the key ingredient of our analysis. We note that according to a formal argument, the residual

uncertainty of the perturbative expansion due to the next-to-leading renormalon contribution is estimated to be $\Lambda_{\rm QCD} \times (a_X \Lambda_{\rm QCD})^2$ for a bound-state X of size a_X [18, 14], e.g. it amounts to 5–20 MeV for the $1S$ bottomonium state. Provided this argument applies, in principle the predictions of perturbative QCD can be made precise down to this accuracy by sufficiently increasing the orders of the perturbative expansion.

The paper is organized as follows. In Sec. 2 we set up the formalism and the computational strategy. In Sec. 3 we perform the numerical analysis and in Sec. 4 we discuss the errors. In Sec. 5 we interpret our result and in Sec. 6 we draw some conclusions.

2 Perturbative Expansions

We assume that the system is non-relativistic, $v \ll 1$, where v is the typical size of the heavy quark velocity in a quarkonium state. Also, we assume that the soft scale mv is much larger than $\Lambda_{\rm QCD}$. Under these assumptions, the energy (mass) of a quarkonium state X is given as a series expansion in the $\overline{\rm MS}$ coupling constant $\alpha_{\rm s}(\mu)$ defined in the theory with n_l massless quarks only. We write a general expression valid also when the masses of the quark and antiquark are different. The reduced mass is defined from the pole masses by $m_r = m_{1,\rm pole} m_{2,\rm pole}/(m_{1,\rm pole} + m_{2,\rm pole})$. Moreover, we define $x = 1 - 4m_r/(m_{1,\rm pole} + m_{2,\rm pole})$; when the two masses are equal, $x = 0$. Up to $\mathcal{O}(\alpha_{\rm s}^4 m)$ the energy of a heavy quarkonium state X, identified by the quantum numbers n, l, s and j, is given by*

$$E_X(\mu, \alpha_{\rm s}(\mu), m_{i,\rm pole}) = m_{1,\rm pole} + m_{2,\rm pole} + E_{{\rm bin},X}(\mu, \alpha_{\rm s}(\mu), m_{i,\rm pole}), \tag{1}$$

$$E_{{\rm bin},X}(\mu, \alpha_{\rm s}(\mu), m_{i,\rm pole}) = -\frac{8}{9n^2}\,\alpha_{\rm s}(\mu)^2 m_r \sum_{k=0}^{2} \varepsilon^{k+1} \left(\frac{\alpha_{\rm s}(\mu)}{\pi}\right)^k P_k(L_{nl}), \tag{2}$$

where $\varepsilon = 1$ is the parameter that will be used in order to properly organize the perturbative expansion in view of the $\mathcal{O}(\Lambda_{\rm QCD})$ renormalon cancellation. $P_k(L_{nl})$ is a k-th-degree polynomial of $L_{nl} \equiv \log[\,3n\mu/(8\alpha_{\rm s}(\mu) m_r)\,] + S_1(n+l) + \dfrac{5}{6}$, and the harmonic sums are defined as $S_p(q) \equiv \displaystyle\sum_{k=1}^{q} \frac{1}{k^p}$. It is convenient to decompose the polynomials into renormalization-group invariant subsets:

$$P_0 = 1, \tag{3}$$

$$P_1 = \beta_0\, L_{nl} + c_1, \tag{4}$$

$$P_2 = \frac{3}{4}\beta_0^2\, L_{nl}^2 + \left(-\frac{1}{2}\beta_0^2 + \frac{1}{4}\beta_1 + \frac{3}{2}\beta_0 c_1\right) L_{nl} + c_2. \tag{5}$$

Here, β_k's denote the coefficients of the QCD beta function, $\beta_0 = 11 - 2n_l/3$, $\beta_1 = 102 - 38n_l/3$, and c_k's are given by

$$c_1 = -4, \tag{6}$$

*The full formula up to $\mathcal{O}(\alpha_{\rm s}^4 m)$ for the S state spectrum was derived in [7] and later confirmed in [9]; additional corrections necessary for the spectrum of $l \geq 1$ states can be found in [16]; the formula for the unequal mass case was derived in [21].

$$
\begin{aligned}
c_2 \;=\; & -\frac{16\,\pi^2\,\{2s(s+1)(1-x)+3x\}}{27\,n}\,\delta_{l0} - \frac{8\,\pi^2\,(D_S+3\,X_{LS})}{9\,n\,l\,(l+1)\,(2\,l+1)}\,(1-\delta_{l0}) + \beta_0^2\,\nu(n,l) \\
& -\frac{(11+x)\,\pi^2}{9\,n^2} + \frac{68\,\pi^2}{9\,n\,(2\,l+1)} + \frac{473}{16} + \frac{9\,\pi^2}{2} + \frac{33\,\zeta_3}{4} - \frac{9\,\pi^4}{32} - n_l\,\left(\frac{109}{72} + \frac{13\,\zeta_3}{6}\right),
\end{aligned}
\tag{7}
$$

with

$$
D_S \equiv \left\langle 3\frac{(\vec{r}\cdot\vec{S})^2}{r^2} - \vec{S}^2 \right\rangle = \frac{2l(l+1)s(s+1) - 3X_{LS} - 6X_{LS}^2}{(2l-1)(2l+3)}, \tag{8}
$$

$$
X_{LS} \equiv \left\langle \vec{L}\cdot\vec{S} \right\rangle = \frac{1}{2}\,\left[j(j+1) - l(l+1) - s(s+1)\right], \tag{9}
$$

$$
\begin{aligned}
\nu(n,l) = {} & \frac{\pi^2}{8} - \frac{1}{2}\,S_2(n+l) + \frac{n}{2}\frac{(n+l)!}{(n-l-1)!}\sum_{k=1}^{\infty}\frac{(n-l+k-1)!}{(n+l+k)!\,k^3} \\
& + \frac{(n-l-1)!}{2(n+l)!}\sum_{k=1}^{n-l-1}\frac{(2l+k)!\,(2k+2l-n)}{(k-1)!\,(k+l-n)^3}.
\end{aligned}
\tag{10}
$$

It is understood that the last term of Eq. (10) is zero if $n-l<2$.[†]

Next we rewrite the series expansion of E_X in terms of the $\overline{\rm MS}$ masses. This is done by expressing the pole masses $m_{i,\rm pole}$ in terms of the renormalization–group-invariant $\overline{\rm MS}$ masses $\overline{m}_i \equiv m_{i,\overline{\rm MS}}(m_{i,\overline{\rm MS}})$:

$$
m_{i,\rm pole} = \overline{m}_i\left\{1 + \frac{4}{3}\varepsilon\frac{\alpha_{\rm s}(\overline{m}_i)}{\pi} + \varepsilon^2\left(\frac{\alpha_{\rm s}(\overline{m}_i)}{\pi}\right)^2 d_1 + \varepsilon^3\left(\frac{\alpha_{\rm s}(\overline{m}_i)}{\pi}\right)^3 d_2\right\}. \tag{11}
$$

The coefficient d_1 is given in [22], while the analytic expression of d_2 can be derived from the result of [23], the renormalization-group evolutions of $\alpha_{\rm s}(\mu)$ and $m_{\overline{\rm MS}}(\mu)$, and the matching condition [24]. Note that the counting in ε in Eq. (2) and Eq. (11) does not reflect the order in $\alpha_{\rm s}$ but the wanted renormalon cancellation. One way to understand this is to consider that in the sum of the pole-quark masses and the static QCD potential, $\sum_i m_{i,\rm pole} + V_{\rm QCD}(r)$, the renormalon cancellation takes place without reordering of power counting in $\alpha_{\rm s}$ [5, 6]. The extra power of $\alpha_{\rm s}$ comes in the energy level expansion when the dynamical variable r^{-1} is replaced by the dynamical scale $\langle nlsj\,|\,r^{-1}\,|\,nlsj\,\rangle \sim C_F\alpha_{\rm s}m_r/n$.[‡] Moreover, in order to realize the renormalon cancellation at each order of the expansion, it is necessary to expand $m_{i,\rm pole}$ and $E_{{\rm bin},X}$ in the same coupling [25, 19, 26], therefore we express $\alpha_{\rm s}(\overline{m}_i)$ in (11) in terms of $\alpha_{\rm s}(\mu)$:

$$
\alpha_{\rm s}(\overline{m}_i) = \alpha_{\rm s}(\mu)\left\{1 + \varepsilon\,\frac{\alpha_{\rm s}(\mu)}{\pi}\,\frac{\beta_0}{2}\log\left(\frac{\mu}{\overline{m}_i}\right) + \varepsilon^2\left(\frac{\alpha_{\rm s}(\mu)}{\pi}\right)^2\,\left[\frac{\beta_0^2}{4}\,\log^2\left(\frac{\mu}{\overline{m}_i}\right) + \frac{\beta_1}{8}\log\left(\frac{\mu}{\overline{m}_i}\right)\right]\right\}. \tag{12}
$$

[†]The infinite sum in Eq. (10) can be easily evaluated analytically in terms of ζ_3, etc. for given values of n and l, e.g. by using *Mathematica*.

[‡]Since the soft scale is, in perturbative QCD, the only scale involved in the calculation of the binding energy, $E_{{\rm bin},X}$, up to $\mathcal{O}(\alpha_{\rm s}^4 m)$, we may absorb the extra $\alpha_{\rm s}$ by reexpressing $E_{{\rm bin},X}$ in terms of $\alpha_{\rm s}(\mu)$ and the soft scales $\mu_{i,\rm soft} = \alpha_{\rm s}(\mu)\,\overline{m}_i$. Then the order counting in $\alpha_{\rm s}(\mu)$ coincides with the order counting in ε given here.

Substituting Eqs. (12) and (11) into Eqs. (2) and (1) we get an expression for the energy levels of the heavy quarkonium states, which depends on μ, $\alpha_{\rm s}(\mu)$ and $\overline{m}_i$, that we can organize as an expansion in ε up to order ε^3:

$$\begin{aligned} E_X(\mu,\alpha_{\rm s}(\mu),\overline{m}_i) &= \overline{m}_1+\overline{m}_2+E_X^{(1)}(\mu,\alpha_{\rm s}(\mu),\overline{m}_i)\varepsilon+E_X^{(2)}(\mu,\alpha_{\rm s}(\mu),\overline{m}_i)\varepsilon^2 \\ &\quad +E_X^{(3)}(\mu,\alpha_{\rm s}(\mu),\overline{m}_i)\varepsilon^3+\ldots \end{aligned} \tag{13}$$

Since the counting in ε explicitly realizes the order $\Lambda_{\rm QCD}$ renormalon cancellation, and since $\alpha_{\rm s}$ and $\overline{m}_i$ are short-range quantities, the obtained perturbative expansion (13) is expected to show a better convergence with respect to the original expansion (2).

The obtained quarkonium mass E_X depends on the scale μ, due to our incomplete knowledge of the perturbative series. We fix the scale μ by demanding stability against variation of the scale:

$$\left.\frac{d}{d\mu}E_X(\mu,\alpha_{\rm s}(\mu),\overline{m}_i)\right|_{\mu=\mu_X}=0. \tag{14}$$

When we do this, we expect that the convergence properties of the series become optimal, and that the scale becomes close to the inverse of the physical size of the bound-state X. If the scale fixed by Eq. (14) evidently does not fulfill these expectations, then the theoretical predictions obtained in this way will be considered *unreliable*. We will show that this typically happens when the coupling constant becomes bigger than one.

Based on the formalism developed in [14], in principle three scenarios are possible under the assumption $v \ll 1$ and $mv \gg \Lambda_{\rm QCD}$: 1) The energy or ultrasoft scale mv^2 is much larger than $\Lambda_{\rm QCD}$. In this case the potential is entirely perturbative and non-perturbative corrections are parameterized by local condensates of the Voloshin–Leutwyler type [20]. 2) The energy scale mv^2 is of order $\Lambda_{\rm QCD}$. The potential is entirely perturbative and non-perturbative corrections are parameterized by non-local condensates. 3) The energy scale, mv^2, is smaller than $\Lambda_{\rm QCD}$. In this case short-range non-perturbative corrections affect the potential. They are parameterized by non-local condensates. A perturbative treatment of the energy levels is consistent only if these are small compared to the Coulomb potential. Explicit formulas for the non-perturbative contributions in all these three cases can be found in [14]. However, their sizes in an actual calculation of the heavy quarkonium spectrum are affected by large uncertainties. The best known case is 1): The leading non-perturbative contribution is $\simeq 1.44\, n^6\langle\alpha_{\rm s}F^2(0)\rangle/(m^3\alpha_{\rm s}(\mu)^4)$. It runs out of control for $n>1$, so the estimate is suitable only for the heavy quarkonium ground states. It is quite sensitive to the value of the gluon condensate and of $\alpha_{\rm s}$. It is also numerically sensitive to the replacement of the strong coupling constant in the $\overline{\rm MS}$ scheme in the denominator with the coupling constant in some other scheme (e.g. the V scheme or similar) as used by some authors [7, 16]. Non-local condensates, which are suitable for the situations 2) and 3), are even less known. Moreover, they get entangled with higher-order perturbative corrections (starting at order $\alpha_{\rm s}^5 m\log\alpha_{\rm s}$ [1]) and in particular with the $\mathcal{O}(\Lambda_{\rm QCD}^3)$ renormalon [14]. Due to these uncertainties a direct evaluation of non-perturbative and higher-order contributions will not be included in the present investigation. Neither we will distinguish among the three different scenarios outlined above. Our approach consists in looking only at

the perturbative spectrum up to $\mathcal{O}(\alpha_s^4 m)$, under the general assumption that $mv \gg \Lambda_{\rm QCD}$. The internal consistency of the perturbative series (i.e. its convergence) and the comparison with the experimental data will provide indirect, but more stringent, contraints on the size of non-perturbative and higher-order corrections.

3 Numerical Analyses

In this section we examine the series expansions of the quarkonium spectra, Eq. (13), numerically. The input value is $\alpha_s^{(5)}(M_Z) = 0.1181$ [27]. We evolve the coupling and match it to the couplings of the theory with $n_l = 4$ and 3 successively following [28][§] and solving the renormalization-group equation numerically (4-loop running). In this section we do not take into account effects of the non-zero charm mass in the $b\bar{b}$ and $b\bar{c}$ systems.

Since we expect the ground states of the $b\bar{b}$ and $c\bar{c}$ systems to be the states less affected by non-perturbative corrections, we fix $\overline{m}_b$ and $\overline{m}_c$ through the conditions

$$E_{\Upsilon(1S)}(\mu_X, \alpha_s(\mu_X), \overline{m}_b) = E^{exp}_{\Upsilon(1S)} = 9.460\,\text{GeV}, \tag{15}$$

$$E_{J/\psi}(\mu_X, \alpha_s(\mu_X), \overline{m}_c) = E^{exp}_{J/\psi} = 3.097\,\text{GeV}, \tag{16}$$

where the experimental values of the vector ground states have been taken from [27]. We assume, for the moment, that this identification is not affected by non-perturbative corrections. From Eqs. (15), (16) and (14) we determine μ_X (see Tab. 1), and the b and c $\overline{\rm MS}$ masses:

$$\overline{m}_b \equiv m_b^{\overline{\rm MS}}(m_b^{\overline{\rm MS}}) = 4.203\ \text{GeV}, \tag{17}$$

$$\overline{m}_c \equiv m_c^{\overline{\rm MS}}(m_c^{\overline{\rm MS}}) = 1.243\ \text{GeV}. \tag{18}$$

These values are in good agreement with recent estimates based on Υ [9, 10] and charmonium [29] sum rules respectively.

Using these masses as input and Eq. (14), we can calculate the energy levels of other observed quarkonium states. These are given in Tab. 1. The series expansions for the charmonium 1^1S_0 state and for the 1^3S_1, 1^3P_j, 2^3S_1, 2^3P_0 and 3^3S_1 bottomonium states converge well. For these states the differences of the theoretical predictions and the experimental data are typically 30–70 MeV. Convergence of the series expansions is poor for the $2P_1$, $2P_2$ and $4S$ bottomonium states as well as for the other charmonium states. We consider that the theoretical predictions for these levels are unreliable and marked the corresponding theoretical predictions with sharps ($\sharp$) in the case of the bottomonium. In the charmonium case unreliable predictions are not displayed. The differences $E_X^{exp} - E_X$ are rather large for the states with sharps. Notice that for these states the corresponding $\alpha_s(\mu_X)$ becomes larger than one, indicating a breakdown of the perturbative series. We also computed the mass of the $B_c(^1S_0)$ state. The theoretical prediction is consistent with the experimental value, although the experimental error is large. Generally, for states, which we consider reliably calculable in the above perturbative approach, the scale dependence decreases as we include more terms of the perturbative series. For states, whose predictions we consider unreliable, the series becomes much more convergent if we would choose a scale different from (typically larger than) μ_X.

[§]We take the matching scales as $\overline{m}_b$ and $\overline{m}_c$, respectively.

State X	E_X^{exp}	E_X	$E_X^{exp} - E_X$	$E_X^{(1)}$	$E_X^{(2)}$	$E_X^{(3)}$	μ_X	$\alpha_{\rm s}(\mu_X)$
J/ψ	3.097	3.097	0	0.362	0.205	0.043	1.07	0.448
$\eta_c(1^1S_0)$	2.980	3.056	-0.076	0.333	0.195	0.042	1.23	0.399
$\Upsilon(1^3S_1)$	9.460	9.460	0	0.837	0.204	0.013	2.49	0.274
$\Upsilon(1^3P_0)$	9.860	9.905	-0.045	1.38	0.115	0.003	1.18	0.409
$\Upsilon(1^3P_1)$	9.893	9.904	-0.011	1.40	0.098	0.002	1.15	0.416
$\Upsilon(1^3P_2)$	9.913	9.916	-0.003	1.42	0.086	0.003	1.13	0.422
$\Upsilon(2^3S_1)$	10.023	9.966	$+0.057$	1.46	0.093	0.009	1.09	0.433
$\Upsilon(2^3P_0)$	10.232	10.268	-0.036	2.37	-0.66	0.15	0.693	0.691
$\Upsilon(2^3P_1)$	10.255	$10.316^\sharp$	$-0.061^\sharp$	3.97	-3.56	1.50	$0.552^\sharp$	1.20
$\Upsilon(2^3P_2)$	10.268	$10.457^\sharp$	$-0.189^\sharp$	4.55	-5.03	2.53	$0.537^\sharp$	1.39
$\Upsilon(3^3S_1)$	10.355	10.327	$+0.028$	2.34	-0.583	0.163	0.698	0.684
$\Upsilon(4^3S_1)$	10.580	$11.760^\sharp$	$-1.180^\sharp$	5.45	-6.47	4.38	$0.527^\sharp$	1.61
$B_c(1^1S_0)$	6.4 ± 0.4	6.324	0.08 ± 0.4	0.668	0.187	0.022	1.64	0.329

Table 1: Comparisons of the theoretical predictions of perturbative QCD and the experimental data. We used $n_l = 4$ for $b\bar{b}$ systems and $n_l = 3$ for $c\bar{c}$ and $b\bar{c}$ systems. All dimensionful numbers are in GeV unit.

The value of μ_X for the 1^3S_1 state of $b\bar{b}$ is close to the central value (2.575 GeV) used in [7], while the value for the 1^3S_1 state of $c\bar{c}$ is lower than the central value (1.57 GeV) used by the same authors. The value of μ_X used in Tab. 1 for the 1^1S_0 state of the $b\bar{c}$ is close to the central value (1.6 GeV) used in [21]. We also notice a remarkable agreement with their value of the B_c mass. This supports the idea that the scale of minimal sensitivity is, indeed, close to the characteristic scale of the system, which may be identified with the inverse of its size.

Fig. 1 compares the experimental values of the bottomonium spectrum with theoretical predictions after eliminating those states, which are not reliably calculable (2^3P_1, 2^3P_2 and 4^3S_1 states). If we take an average of the S-wave and P-wave levels corresponding to each principal quantum number n, the theoretical predictions with $\alpha_{\rm s}(M_Z) = 0.1181$ reproduce the experimental values fairly well. On the other hand, the predictions for the S–P splittings and the fine splittings are smaller than the experimental values.

4 Error Estimates

Besides non-perturbative corrections, there are three different kinds of uncertainties in our theoretical predictions for the quarkonium spectra, listed below and in Tab. 2. We examine them separately. Also these examinations indicate that the theoretical predictions for the 2^3P_1, 2^3P_2 and 4^3S_1 bottomonium states are quite unstable, while the prediction for the 2^3P_0 state is at the boundary.

1) *Uncertainty of* $\alpha_{\rm s}^{(5)}(M_Z)$. We analyzed the quarkonium spectra varying the input parameter within the range given in [27]: $\alpha_{\rm s}^{(5)}(M_Z) = 0.1181 \pm 0.0020$. The level spacings become wider for larger $\alpha_{\rm s}^{(5)}(M_Z)$, which is consistent with our naive expectation. We find that the central value $\alpha_{\rm s}^{(5)}(M_Z) = 0.1181$ reproduces the whole level structure better

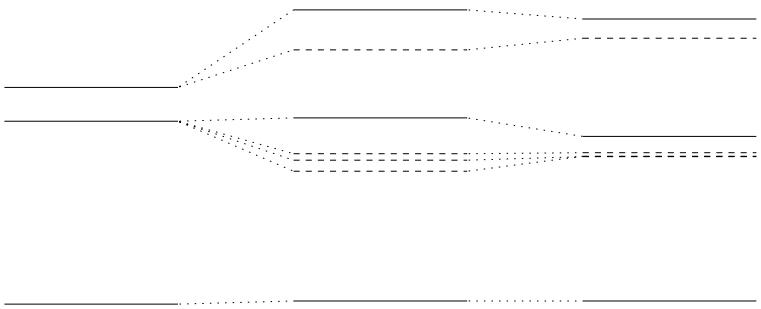

Figure 1: The bottomonium level structure as given by a pure Coulombic potential, by experiments and by the present analysis: the solid and dashed lines represent the S-states and P-states, respectively. The input parameter of the perturbative QCD calculation is $\alpha_{\rm s}^{(5)}(M_Z) = 0.1181$ (see Tab. 1). We show only those levels that we can compute reliably. The Coulomb levels are calculated with $m_{\rm pole} = 5.105$ GeV and $\alpha_{\rm s} = 0.5752$ such that they reproduce the $1S$ and $2S$ levels.

than $\alpha_{\rm s}^{(5)}(M_Z) = 0.1201$ or 0.1161.

2) *Charm Mass Effects.* We have also made an analysis of the bottomonium spectrum including finite charm mass effects. Since they deserve a detailed analysis of their own, including new calculations, we will report the full results in a separate paper [30]. Here we only summarize some of the qualitative features of the effects and include them as a part of the uncertainties of our present analysis. The corrections to the reliable predictions turn out to be positive and to become larger for higher states, ranging up to ~ 200 MeV. Much of the effects, however, may be reabsorbed by the uncertainties in $\alpha_{\rm s}^{(5)}(M_Z)$ (as given above).¶

3) *Uncertainties from Higher-Order Corrections.* We take the maximum value of the following five estimates as an estimate of uncertainties from unknown higher-order corrections for each series expansion: (i) The difference between the theoretical predictions computed using $\alpha_{\rm s}(\mu)$ as obtained by solving the renormalization-group equation perturbatively at 4 loops (Eqs. (3) and (11) of Ref. [28]) and numerically at 4 loops (the data of Tab. 1). (Note that the number of energy levels that can be determined in a reliable way is larger with the former definition of the running coupling constant. Also in that case, reliable predictions turn out to be close to the experimental values.) (ii) The difference between the theoretical predictions computed using the 3-loop and the 4-loop (as in Tab. 1) running coupling constants, fixing $\alpha_{\rm s}^{(5)}(M_Z) = 0.1181$. (iii) The difference between the theoretical estimates obtained by fixing μ_X on the minimum of $|E^{(3)}|$ and the results of Tab. 1, obtained by fixing μ_X via the condition (14). (iv) The contribution $\pm|E_X^{(3)}|$ from Tab. 1. (v) For the $1S$ states we consider the $\mathcal{O}(\alpha_{\rm s}^5 m)$ corrections calculated in the large-β_0 approximation in [3].

¶We note that the sensitivities of the higher levels to a variation of $\alpha_{\rm s}^{(5)}(M_Z)$ increase by the charm mass effects due to the decoupling of the charm quark.

For comparison, we list more conservative error estimates. These are the variations of $\overline{m}_{b,c}$ and E_X when we fix the scale as twice[‖] of the minimal sensitivity scale: $\mu = 2\mu_X$, where μ_X is determined from Eq. (14).

		$\delta\alpha_{\rm s}^{(5)}(M_Z)$	Estimates of higher-order corrections						
		$= \pm 0.0020$	(i)	(ii)	(iii)	(iv)	(v)	$\pm$max	$\mu = 2\mu_X$
$\delta\overline{m}_b$		$^{-19}_{+18}$	-2	$+1$	0	± 7	$+5$	± 7	$+16$
$\delta\overline{m}_c$		$^{-16}_{+15}$	-5	$+4$	$+3$	± 21	$+20$	± 21	$+37$
δE_X	$\Upsilon(1^3P_0)$	$^{+54}_{-48}$	$+15$	-14	0	± 3		± 15	-53
	$\Upsilon(1^3P_1)$	$^{+63}_{-42}$	$+22$	-8	$+7$	± 2		± 22	-48
	$\Upsilon(1^3P_2)$	$^{+57}_{-50}$	$+16$	-16	0	± 3		± 16	-54
	$\Upsilon(2^3S_1)$	$^{+65}_{-58}$	$+18$	-19	-1	± 9		± 19	-73
	$\Upsilon(2^3P_0)$	$^{+117}_{+755^\sharp}$	$+33$	-57	-21	± 150		± 150	-120
	$\Upsilon(2^3P_1)$	$^{+83^\sharp}_{+1189^\sharp}$	-4	$+1637^\sharp$	$-66^\sharp$	$\pm 1500^\sharp$		$\pm 1637^\sharp$	-97
	$\Upsilon(2^3P_2)$	$^{-44^\sharp}_{+1528^\sharp}$	-136	$+2136^\sharp$	$-206^\sharp$	$\pm 2530^\sharp$		$\pm 2530^\sharp$	-229
	$\Upsilon(3^3S_1)$	$^{+130}_{-93}$	$+37$	-63	-36	± 163		± 163	-161
	$\Upsilon(4^3S_1)$	$^{-381^\sharp}_{+1883^\sharp}$	$-639^\sharp$	$+2936^\sharp$	$-1425^\sharp$	$\pm 4380^\sharp$		$\pm 4380^\sharp$	-1361
	$B_c(1^1S_0)$	$^{+4}_{-5}$	-4	0	-1	± 22		± 22	$+1$

Table 2: Variations of the theoretical predictions of Tab. 1 when the uncertainties 1) and 3) discussed in Sec. 4 are separately taken into account. All dimensionful numbers are in MeV unit. Those values corresponding to the unreliable theoretical predictions are marked with sharps. The input parameter is taken as $\alpha_{\rm s}(M_Z) = 0.1181$ except in the first column. The column "$\pm$max" lists $\pm\max\{|(\mathrm{i})|, |(\mathrm{ii})|, |(\mathrm{iii})|, |(\mathrm{iv})|, |(\mathrm{v})|\}$. In the last column we write conservative estimates with the scale choice $\mu = 2\mu_X$.

5 Interpretation

The most non-trivial feature of the present theoretical predictions for the bottomonium spectrum is that the level spacings between consecutive n's are almost constant, whereas in the Coulomb spectrum the level spacings decrease as $1/n^2$.[*] Conventionally, this same difference between the Coulomb spectrum and the observed quarkonium spectra motivated people to construct various potential models. It is, therefore, imperative to elucidate how the above perturbative QCD calculation is able to reproduce such a level structure. We will focus on two points: (1) the leading renormalon cancellation, which implies that infrared physics decouples; this is essential to obtain convergent series expansions; (2) the meaning of the scale μ_X chosen by the scale-fixing prescription (14).

[‖]If we fix the scale as half of the minimal sensitivity scale, $\mu = \mu_X/2$, the predictions for the $n = 2$ bottomonium states appear to be meaningless, since the scales are quite close to the infrared singularity of the runnning coupling constant, and the predictions for the $n \geq 3$ states do not exist, since the scales lie below the infrared singularity.

[*]If we consider, for instance, the ratio $(E_{3S} - E_{2S})/(E_{2S} - E_{1S})$, then we obtain experimentally 0.59, from the data of Tab. 1, 0.71, while from a pure Coulomb interaction 0.19.

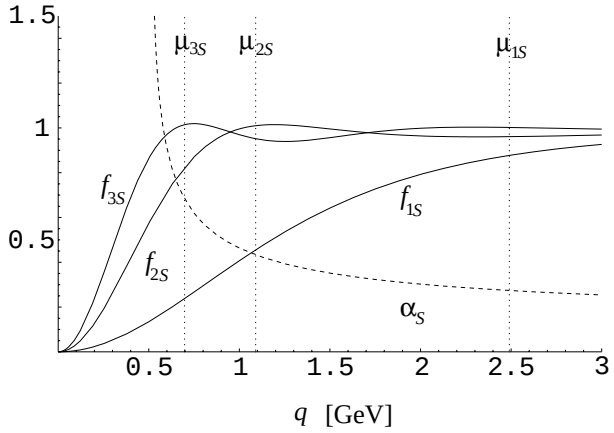

Figure 2: The support functions $f_X(q)$ vs. q for $X = 1S$, $2S$ and $3S$ (solid lines). $f_X(q)$ is calculated using $m_{\rm pole} = 5$ GeV and a different $\alpha_{\rm s}(\mu_X)$, taken from Tab. 1, for each X. Vertical lines represent the corresponding scales μ_X taken from the same table. Also $\alpha_{\rm s}^{(4)}(q)$ is shown by a dashed line.

Let us approximate each term on the right-hand-side of Eq. (1) (in the equal-mass case) as

$$2m_{\rm pole} \simeq 2\overline{m} + \int\limits_{|\vec{q}|<\overline{m}} \frac{d^3\vec{q}}{(2\pi)^3}\,|V_{\rm QCD}(q)| = 2\overline{m} + \frac{2C_F}{\pi}\int_0^{\overline{m}} dq\,\alpha_V(q), \tag{19}$$

$$E_{{\rm bin},X} \simeq \langle X\,|\,\frac{\vec{p}^{\,2}}{m_{\rm pole}} + V_{\rm QCD}\,|\,X\,\rangle\,. \tag{20}$$

Here, $V_{\rm QCD}(q) = -C_F 4\pi\alpha_V(q)/q^2$ is the QCD static potential in momentum space; $|\,X\,\rangle$ denotes the Coulomb wave function (the zeroth-order approximation) and $C_F = 4/3$. The first approximation follows from the fact that the dominant contribution to the pole-$\overline{\rm MS}$ mass relation can be read from the infrared region, loop momenta $q \ll \overline{m}$, of the QCD static potential [6]. The second approximation is more obvious. Let us note that also the right-hand-side of Eq. (20) incorporates and is dominated by the leading renormalon contribution to the static potential. From Eqs. (19) and (20) we obtain

$$E_X \simeq 2\overline{m} + \frac{2C_F}{\pi}\int_0^\infty dq\,\alpha_V(q)\,f_X(q) + \langle X\,|\,\frac{\vec{p}^{\,2}}{m_{\rm pole}}\,|\,X\,\rangle \simeq 2\overline{m} + \frac{2C_F}{\pi}\int_0^\infty dq\,\alpha_V(q)\,f_X(q). \tag{21}$$

The last approximation follows from the fact that the kinetic energy contribution to the bottomonium levels turns out to be numerically small[†] (notice that this does not contradict the virial theorem, since the static potential we are considering here incorporates the running of $\alpha_{\rm s}$ and therefore is not simply of the form $1/r$). The support function f_X is

$$f_X(q) = \theta(\overline{m} - q) - \int_0^\infty dr\,r^2|R_X(r)|^2\,\frac{\sin(qr)}{qr}, \tag{22}$$

where $R_X(r)$ is the radial part of the Coulomb wave-function of X. $f_X(q)$ is almost unity in the region $1/a_X \lesssim q < \overline{m}$, where a_X is the inverse of the dumping scale of f_X and may

[†]It is about 17% of $E_X^{(1)}$ for the $X = 1S$ state, 6% of $E_X^{(1)}$ for the $X = 2S$ state, 4% of $E_X^{(1)}$ for the $X = 3S$ state. Moreover, these contributions tend to cancel each other in the level spacings.

be interpreted as the size of the bound-state X.[‡] For the $1S$ state $f_X(q)$ dumps slowly as q decreases. For other states $f_X(q)$ dumps rapidly from scales which are somewhat smaller than the naive expectations $(C_F\alpha_s m_{\rm pole})/n_X$. Eq. (21) tells that *the major contribution to the energy levels comes from the region* $1/a_X \lesssim q \lesssim \overline{m}$ *of the self-energy corrections of quark and antiquark* (apart from the constant contribution $2\overline{m}$). In Fig. 2 we show f_X for different states calculated with $m_{\rm pole} = 5$ GeV and $\alpha_s(\mu_X)$ taken from Tab. 1. The corresponding values of μ_X are also displayed. For those states which we consider the predictions reliable, μ_X is located within the range where $f_X(q) \simeq 1$ (close to the infrared edge); for those states with unreliable predictions, μ_X is located out of this range but far in the infrared region. In Fig. 2 also $\alpha_s(q)$ is shown. We see that as n_X increases from 1 to 3, the coupling $\alpha_s(q)$, close to the dumping scale of $f_X(q)$, grows rapidly. According to Eq. (21), this is the very reason for the widening of the level spacings in excited states in comparison to the Coulomb spectrum.

Summarizing the above discussion we may draw the following qualitative picture of the structure of the bottomonium spectrum:

- The energy levels of bottomonium are mainly determined by (i) the $\overline{\rm MS}$ masses of b and $\bar{b}$, and (ii) contributions to the self-energies of b and $\bar{b}$ from gluons with wavelengths $1/\overline{m} \lesssim \lambda \lesssim a_X$. The latter contributions may be regarded as the difference between the (state-dependent) constituent quark masses and the current quark masses.

- Level spacing between consecutive n's increases rapidly with n as compared to the Coulomb spectra. This is because the self-energy contributions (ii) grow rapidly as the physical size of the bound-state increases.

6 Conclusions

For all the bottomonium states, where the predictions of perturbative QCD can be made reliably (i.e. $\alpha_s < 1$), our results are consistent with the experimental data within the estimated uncertainties of the theoretical predictions. The obtained value for $\overline{m}_b$ is in good agreement with the recent sum-rule calculations. The theoretical uncertainties given in Tab. 2 are numerically of the same size as $\Lambda_{\rm QCD} \times (a_X\Lambda_{\rm QCD})^2$, i.e. of the effect of the $\mathcal{O}(\Lambda^3_{\rm QCD})$ renormalons: if we approximate $1/a_X \simeq \mu_X$, take the values of Tab. 1, and $\Lambda_{\rm QCD} = 300 - 500$ MeV, we obtain for the $1S$ state a contribution of order $\pm(5-20)$ MeV, for the $n = 2$ states a contribution of order $\pm(20 - 110)$ MeV and for the $3S$ state a contribution of order $\pm(50 - 250)$ MeV. Since the mass $\overline{m}_b$ has been fixed on the vector ground state and has *not* been adjusted for higher states, the data at our disposal suggest that: 1) the bulk of the bottomonium spectrum is accessible by perturbative QCD up to some of the $n = 3$ states; 2) non-perturbative contributions do not need to be larger than 250 MeV for the reliable $n = 3$ states, than 100 MeV for the $n = 2$ states and than 20 MeV for $\overline{m}_b$ and may be of the type associated with the $\mathcal{O}(\Lambda^3_{\rm QCD})$ renormalon. These upper bounds to the non-perturbative corrections are conservative and their true sizes

[‡]According to Eq. (21), $1/a_X$ acts as an infrared cut off in the computation of the energy level. We may compare it with a qualitative picture where the gluons, whose wavelengths are much larger than the size of the color-singlet bound-state, cannot couple to it.

may be considerably smaller; note that for reliable predictions all of $|E_X^{exp} - E_X|$ in Tab. 1 are smaller than 80 MeV. The existence of non-perturbative corrections of the above sizes may also explain the discrepancy observed in Tab. 1 between the theoretical estimates and the experimental data of the fine structure and the $2S$-$1P$ splittings. However, before making any definitive statement, an analysis including higher-order corrections is necessary.

The reliability of the perturbative calculations and the agreement with the experimental data indicates that the assumptions made at the end of Sec. 2 are, indeed, satisfied by the $n = 1$, $n = 2$ and some of the $n = 3$ bottomonium states. Hence, non-perturbative contributions are encoded into non-local condensates, which may reduce to local ones for the ground states. These are expected to reabsorb the $\mathcal{O}(\Lambda^3_{\rm QCD})$ renormalon [14] and are of the order $\Lambda_{\rm QCD} \times (a_X \Lambda_{\rm QCD})^2$. The agreement noticed above, between this estimate and the uncertainties of the perturbative series given in Tab. 2, shows the consistency of our conclusions.

For what concerns the $c\bar{c}$ system, with the present method we are not in the condition to make reliable predictions for states higher than the ground state, and, therefore, we cannot extrapolate from consistency arguments the size (and the nature) of the non-perturbative corrections. We have noticed, however, that our estimate for $\overline{m}_c$ is in good agreement with recent sum-rule calculations. From the prediction of the η_c mass we may guess non-perturbative contributions to be, in this case, of the order of 100 MeV. Also this figure is consistent with the $\mathcal{O}(\Lambda^3_{\rm QCD})$ renormalon effect ($20 - 110$ MeV).

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