Fine and Hyperfine Splittings of Charmonium and Bottomonium: An Improved Perturbative QCD Approach

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Abstract

We extend the formalism based on perturbative QCD that was developed in our previous work, and compute the hyperfine splittings of the bottomonium spectrum as well as the fine and hyperfine splittings of the charmonium spectrum. All the corrections up to $\mathcal{O}(\alpha_5^2 m)$ are included in the computations. We find agreement (with respect to theoretical uncertainties) with the experimental values whenever available and give predictions for not yet observed splittings.
Theoretical predictions of the spectra of heavy quarkonia have traditionally been based on phenomenological models for the inter-quark potential that are not a priori connected to fundamental QCD parameters [1, 2]. With suitable model potentials, very good agreement with the observed spectra can be obtained for the charmonium and bottomonium states (e.g. [3]). These studies established the non-relativistic nature of the heavy quarkonium systems and, in overall, a unified shape of the inter-quark potential in the distance region $0.5 \lesssim r \lesssim 5$ GeV$^{-1}$. More recently, lattice computations of the static QCD potential gave a potential shape consistent with the phenomenological potentials in this region [4]. Quarkonium spectra have also been calculated in lattice QCD [5, 6]. In recent calculations of the heavy quarkonium spectra on anisotropic lattices [7–9], reasonably good agreement with experimental values is obtained. In general, lattice calculations still suffer from uncertainties related to the continuum extrapolation and the quenched approximation.

Recent progress in perturbative QCD has drastically improved the description of heavy quarkonium states within perturbative QCD. The essential aspect is that the sum of the QCD potential and the quark-antiquark pole masses, $E_{\text{tot}}(r) = 2m_{\text{pole}} + V_{\text{QCD}}(r)$, can be predicted much more accurately perturbatively in the distance region relevant to heavy quarkonium states [10–13], once the leading-order renormalons are cancelled [14]. In [15, 16] the whole structure of the bottomonium spectrum up to $\mathcal{O}(\alpha_5^4 m)$ was predicted within perturbative QCD taking into account the cancellation of the leading-order renormalons, and a good agreement with the experimental values has been found for the gross structure of the spectrum. Subsequently, in [17] we developed a specific formalism based on perturbative QCD and examined predictions for the bottomonium spectrum. We included in the zeroth-order Hamiltonian the static QCD potential computed in [12], which takes into account cancellation of the renormalons. We have included all the corrections up to $\mathcal{O}(\alpha_5^2 m)$ for the fine splittings and all the corrections up to $\mathcal{O}(\alpha_5^2 m)$ for the individual energy levels. It was shown that good agreement between the computed and the observed bottomonium spectrum can be obtained, including the fine splittings. These analyses [15–17] have shown that the predictions agree with the corresponding experimental data within the estimated perturbative uncertainties, and that the size of non-perturbative contributions is compatible with the size of perturbative uncertainties. (Similar conclusions have been drawn in the analyses of the perturbative QCD potential [10–13].)

In this paper we extend our previous analysis [17] and predict the hyperfine splittings of the bottomonium spectrum including all the corrections up to $\mathcal{O}(\alpha_5^5 m)$. We also predict the fine splittings and hyperfine splittings of the charmonium spectrum including all the corrections up to the same order and using the same QCD potential as used for the bottomonium spectrum. The calculations of the bottomonium hyperfine splittings constitute predictions of the yet unobserved states. An essential difference of our predictions from those of the conventional potential models is as follows: All our predictions are constructed from the ingredients of perturbative QCD. Although our predictions will depend on details of the prescriptions adopted in our formalism, we can identify unambiguously, within the frame of perturbative QCD, which higher order corrections are incorporated in our predictions, hence we may estimate the sizes of the uncertainties originating from the higher-order corrections not included in our computations. As a result, we are able to test the validity of perturbative QCD (within the prescriptions of our formalism), by comparing our predictions with the experimental data with respect to the
estimated uncertainties. This is not the case for the conventional potential models, where their core potentials follow from simple ansätze.

It is not our intention to compete with treatments like [3] in terms of agreement with experiment. Rather than constructing a very special model potential to reproduce experimental spectra, we will show that our predictions can successfully describe the observed quarkonium states (and make stable predictions for yet unobserved states), and that, consequently, perturbative QCD is compatible with the experimental data with essentially only the quark masses and the strong coupling constant as the input parameters.

In general, where the masses of bottomonium and charmonium states have been measured, the experimental uncertainties are much smaller than the theoretical uncertainties [18]. The only two exceptions are the very poorly measured masses of $\eta_b(1S)$ and $\eta_c(2S)$. The mass of $\eta_c(2S)$ had been given as $3594 \pm 5 \text{ MeV}$ [19] for more than 20 years, before a new value of $3654 \pm 6 \pm 8 \text{ MeV}$ was reported by Belle last summer [20].

For the reader’s convenience, let us briefly summarise the formalism used in our previous analysis for the bottomonium spectrum [17]. (The reader is referred to this paper and references therein for technical details and an explanation of the motivation for this choice.)

1. We adopt a special organisation of the perturbative series. The zeroth-order part of the Hamiltonian is chosen as $H_0 = \bar{p}^2/(2m_{\text{pole}}) + 2m_{\text{pole}} + V_{\text{QCD}}(r)$, and all other operators in the Hamiltonian are treated as perturbations.

2. In $H_0$, we replace $2m_{\text{pole}} + V_{\text{QCD}}(r)$ by $E_{\text{imp}}(r)$, which is determined separately in three regions of $r$: in the intermediate-distance region, $E_{\text{imp}}(r)$ is identified with $2m_{\text{pole}} + V_{\text{QCD}}(r)$ up to $O(\alpha_3^3)$, together with a specific prescription for fixing the renormalisation scale $\mu = \mu_2(r)$; in the short-distance region, $E_{\text{imp}}(r)$ is identified with a three-loop renormalisation-group improved potential; in the long-distance region a linear extrapolation is used.

3. As for perturbation, we include all the $O(1/c^2)$ operators; also some of the $O(1/c^3)$ operators are included, in particular, all those operators which contribute to the $O(\alpha^5_3 m)$ corrections to the fine splittings are included.

4. Our predictions depend on the renormalisation scale $\mu$ (for the $\overline{\text{MS}}$ coupling constant), which enters the $O(1/c^2)$ and $O(1/c^3)$ operators. On the other hand, $E_{\text{imp}}(r)$ in the zeroth-order Hamiltonian is constructed such that it is independent of $\mu$, or, its $\mu$-dependence has been removed using a specific scale-fixing prescription. In this way, we take into account a large difference of the scales involved in the individual energy levels and in the level splittings.

In this work the following points are changed as compared to the above formalism.

I. Instead of the linear extrapolation, the long-distance part ($r > r_{\text{IR}} = 4.5 \text{ GeV}^{-1}$) of $E_{\text{imp}}(r)$ is identified with $2m_{\text{pole}} + V_{\text{QCD}}(r)$ up to $O(\alpha_3^3)$, with the scale $\mu$ fixed to that of the intermediate-distance part at $r = r_{\text{IR}}$, i.e. $\mu = \mu_2(r_{\text{IR}})$. 

(II) In addition to the $\mathcal{O}(1/c^3)$ operators considered in [17], we include $\mathcal{O}(1/c^3)$ spin-dependent operators
\begin{align*}
\delta U_0^{(1)} &= \frac{16\pi\alpha_s}{9m_s^2} s (s + 1) \delta^3(\vec{r}) \frac{\alpha_s}{\pi} \left( \frac{23}{12} - \frac{3}{4}\log 2 - \frac{5}{18}n_f \right), \\
\delta U_0^{(2)} &= \frac{16\pi\alpha_s}{9m_s^2} s (s + 1) \frac{\alpha_s}{\pi} \left[ \frac{21}{4} X(r, m) - \frac{\beta_0}{2} X(r, \mu) \right],
\end{align*}
where $\beta_0 = 11 - \frac{2}{3}n_f$, and $\gamma_E = 0.5772\ldots$ is the Euler constant; $n_f$ is the number of active quark flavours.\(^*\) The momentum-space representation of these operators can be found in [21]. These operators contribute to the hyperfine splittings at $\mathcal{O}(\alpha_s^5 m_b)$, whereas they do not affect the fine splittings at this order.

(III) We also compute the fine splittings and hyperfine splittings of the charmonium spectrum using the same formalism. As for the QCD potential, we use the potential constructed for the bottomonium $E_{\text{imp}}(r)$, whose essential part is given by $E_{\text{tot}}^{bb}(r) = V_{\text{QCD}}(r) + 2m_{b,pole}$.\(^†\) The potential, $E_{\text{tot}}(r) = V_{\text{QCD}}(r) + 2m_{p}p_{pole}$, is in principle independent of the quark masses (apart from an $r$-independent constant). But it was shown in [12, 22] that the use of our specific scale-fixing prescription introduces a dependence on the quark mass. It was shown that (by coincidence) the potential becomes most stable for masses of the order of the $b$ quark mass. On the other hand, it turns out to be poorly stable for the charm quark mass. Furthermore, we confirmed that the potentials corresponding to different values of quark masses agree with one another within the estimated theoretical uncertainties. We therefore use the potential as constructed with the $b$ quark mass both for bottomonium and charmonium.

Numerically effects of the change (I) are very small, since the fine and hyperfine splittings are determined predominantly by the short-distance part of the potential. (The last digit of every number listed in Tab. III varies at most by one.) Nevertheless, conceptually, $E_{\text{imp}}(r)$ is now determined by perturbative QCD (in a certain prescription) at every $r$. In particular, we know exactly which higher order corrections are incorporated in $E_{\text{imp}}(r)$ at every $r$. Therefore, we can estimate effects of the higher order corrections not included in our calculations, by changing prescriptions or by including specific types of corrections.

\(^*\)For numerical evaluation, we use the following formula, obtained via integration by parts and the Schrödinger equation with respect to the zeroth-order Hamiltonian:
\begin{align*}
\frac{\int d^3\vec{x} |\psi(\vec{x})|^2 X(r, \sigma)}{\int d^3\vec{x} |\psi(\vec{x})|^2} &= \frac{\int_0^\infty dr \frac{r}{2\pi} \left[ m \left\{ V(r) + \frac{i(l+1)}{mr^2} - E \right\} |R_i(r)|^2 + |R_i'(r)|^2 \right] \{\log(\sigma r) + \gamma_E\} }{\int_0^\infty dr r^2 |R_i(r)|^2 },
\end{align*}
where $\psi(\vec{x}) = R_i(r) Y_{lm}(\theta, \phi)$ denotes an unnormalised zeroth-order wave function.

\(^†\)The charmonium level splittings computed in this paper are not affected by an $r$-independent constant to be added to $E_{\text{imp}}(r)$. In calculating the whole charmonium spectrum, we may fix the $r$-independent constant e.g. by matching the computed $J/\psi$ mass to the experimental value.
Level splitting

|                  | Exp. | Potential model | Lattice | Pert. QCD based |
|------------------|------|-----------------|---------|-----------------|
|                  |      | [2] [3] [23] [24] [9] [8] [25] this work |
| \( \chi_{c1}(1P) - \chi_{c0}(1P) \) | 95   | 50 81 86 72     | 79  -  -      | 56   |
| \( \chi_{c2}(1P) - \chi_{c1}(1P) \) | 46   | 21 50 46 49     | 35  -  -      | 43   |
| \( J/\Psi - \eta_c(1S) \) | 117  | 117 117 117 117 | 85  -  -      | 88   |
| \( \Psi(2S) - \eta_c(2S) \) | 92/32| 78 72 98 92     | 43  -  -      | 38   |
| \( \chi_{c}^{\text{cog}}(1P) - h_{c}(1P) \) | -0.9 | 0 0 0 9         | 1.5 - -1.4   | -0.8 |
| \( \Upsilon(1S) - \eta_b(1S) \) | (160)| 87 57 60 45     | -51 - -      | 44   |
| \( \Upsilon(2S) - \eta_b(2S) \) | -    | 44 28 30 28     | -  -  -      | 21   |
| \( \Upsilon(3S) - \eta_b(3S) \) | -    | 41 20 27 23     | -  -  -      | 12   |
| \( \chi_{b}^{\text{cog}}(1P) - h_{b}(1P) \) | -    | 0 0 -1 1        | -  - -0.5    | -0.4 |
| \( \chi_{b}^{\text{cog}}(2P) - h_{b}(2P) \) | -    | 0 0 -1 0        | -  - -0.4    | -0.2 |

Table 1: Fine and hyperfine splittings of the charmonium spectrum and hyperfine splittings of the bottomonium spectrum. All values in MeV. In models [2,3], no interaction has been incorporated that produces the \( 3P_1 \) hyperfine splittings. As for the results of [9], we quote the values from Table 10 of that paper. In [25] the matrix elements of \( X(r,m) \) and \( X(r,\mu) \) in eq. (2) were extracted from the experimental values for the fine splittings instead of computing them from perturbative QCD.

In Tab. 1 we list our predictions for the fine splittings and the hyperfine splittings of the charmonium spectrum as well as the hyperfine splittings of the bottomonium spectrum. Only the states below the threshold for strong decays \( 2m_D = 3729 \text{ MeV} \) and \( 2m_B = 10558 \text{ MeV} \) are considered. \( \chi_{c,b}^{\text{cog}} \) denotes the centre of gravity of the triplet \( P \)-wave states (the spin-averaged \( 3P_J \) mass with the weight factor \( 2J+1 \)). The input parameters of our predictions are \( \alpha_s(M_Z) = 0.1181 \), \( m_{b}^{\text{MS}}(m_{c}^{\text{MS}}) = 4190 \text{ MeV} \) [16], \( m_{c}^{\text{MS}}(m_{c}^{\text{MS}}) = 1243 \text{ MeV} \) [15], and \( \mu = 1.5 \) (3) GeV, \( n_t = 3 \) (4) for charmonium (bottomonium). For comparison we list the corresponding experimental values, some model predictions, and predictions from recent lattice computations. Our predictions for the bottomonium fine splittings have already been presented in [17].

We see that the level of agreement of our predictions with the experimental values is comparable to that of the recent lattice results.\(^4\) On the other hand, generally the potential models reproduce the experimental values much better. This feature would be understandable, since the potential models contain much more input parameters than the lattice or our predictions. As we will discuss below, our predictions are consistent with the experimental values with respect to estimated theoretical uncertainties. The same is true for the lattice results. On the other hand, generally it is difficult to estimate errors of the theoretical predictions of the potential models (without comparing to experimental values), as there are no systematic ways to improve accuracies of their predictions.

\(^4\)It should be noted, however, that qualitatively quite different kinds of theoretical errors are contained in the lattice computations [9,8] and our computations. For instance, the former are performed in the quenched approximation, whereas the latter include the sea quark effects fully; the latter computations are subject to relativistic corrections, whereas the former computations are carried out fully relativistically.
As for the splitting $\Psi(2S) - \eta_c(2S)$ in Tab. 1, all the model calculations try to reproduce the old experimental value, while the lattice calculation and our calculation favour the new value. Note that, even if we take unrealistic values for the input parameters of our calculations ($\alpha_S(M_Z)$, $m_c^{\overline{MS}}(m_c^{\overline{MS}})$, $\mu$), we cannot magnify only the splitting $\Psi(2S) - \eta_c(2S)$ while keeping other splittings almost unchanged.

It has been emphasised [26] that the sizes and the signs of the $3P_{cog} - 1P_{1}$ hyperfine splittings can distinguish various models, since there exists wide variation of theoretical predictions for this quantity presently. In particular, [25] predicted the $3P_{cog} - 1P_{1}$ hyperfine splittings using a relation between these splittings and the fine splittings derived from perturbative QCD. Our predictions are consistent with their values within theoretical errors. The difference is that we predict the matrix elements of $X(r,m)$ and $X(r,\mu)$ in eq. (2) from the input quark masses and the strong coupling constant. In perturbative QCD, the $3P_{cog} - 1P_{1}$ hyperfine splittings are generated first at $O(\alpha_s^3 m)$, whereas the fine splittings and the $S$-state hyperfine splittings are of $O(\alpha_s^4 m)$. For this reason, and also due to some small overall coefficient, the former splittings are predicted to be much smaller than the latter splittings within perturbative QCD [25]. Some potential models do not possess this property, as discussed in [26].

The inclusion of the $O(1/c^3)$ operators makes our results fairly scale–independent over a remarkably wide range of scales, a property that was already emphasised for the bottomonium fine splittings in our previous work. We consider this stability against scale variations an important indication of the reliability of our formalism. We show the scale dependences of the splittings in Tab. 2.

![Table 2](image)

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We examine several sources of theoretical uncertainties of our predictions in Tab. 3. Individual errors (i)–(iv) are estimated as follows. (Unless stated otherwise explicitly, the same input parameters as in Tab. 1 are used.)

(i) Variation of our prediction when $\alpha_S(M_Z)$ is changed from 0.1181 to 0.1161 (left column) or to 0.1201 (right column).
Table 3: Error estimates of our predictions. See text for explanations on the individual error estimates (i)–(iv). As a combined error, \( \sqrt{(i)^2 + \text{Max}[(ii), (iii), (iv)]^2} \) is listed. “diff. from exp.” denotes the difference between our prediction, given in Tab. 4, and the experimental value.

(ii) Variation of our prediction when the potential \( E_{\text{imp}}(r) \) is replaced by \( E_{\text{imp}}(r) + \frac{1}{2} \Lambda^3 r^2 \) \( (\Lambda = 300 \text{ MeV}) \). According to the analysis [12] of \( E_{\text{imp}}(r) \) (see also [22]), this can be used as an estimate of the error induced by uncertainties of the potential.

(iii) Variation of our prediction when the scale \( \mu \) is varied by a factor of two (between 1–2 GeV for charmonium and 2–4 GeV for bottomonium).

(iv) The size of the next-to-leading order corrections of our prediction (within our organisation of the perturbative expansion). The next-to-leading order corrections to the \( ^3P_{\text{cog}} - ^1P_1 \) hyperfine splittings are not yet known.

Of these, (ii)–(iv) can be regarded as estimates of the sizes of higher-order corrections. We have also checked that errors induced by uncertainties of the input \( m_{b,\text{MS}}(m_{b,\text{MS}}) \) and \( m_{c,\text{MS}}(m_{c,\text{MS}}) \) are negligible compared to the above error estimates, where we varied \( m_{b,\text{MS}}(m_{b,\text{MS}}) \) and \( m_{c,\text{MS}}(m_{c,\text{MS}}) \) by 50 and 100 MeV, respectively.

As combined errors, \( \sqrt{(i)^2 + \text{Max}[(ii), (iii), (iv)]^2} \) are listed. Comparing them with the differences of our predictions from the experimental values, for charmonium, we find a reasonable agreement of our predictions and the experimental values with respect to the estimated errors. Furthermore, the values of the combined errors are consistent with the error estimates, which can be obtained following the logic employed for estimating theoretical uncertainties of the bottomonium fine splittings in [17]: order \( \Lambda_{\text{QCD}}^3/m_c^2 \approx 10–50 \text{ MeV} \) for the charmonium fine and hyperfine splittings and order \( \Lambda_{\text{QCD}}^3/m_b^2 \approx 1–10 \text{ MeV} \) for the bottomonium hyperfine splittings, except for the \( ^3P_{\text{cog}} - ^1P_1 \) hyperfine splittings.

To conclude, we find that our formalism gives predictions for the charmonium fine and hyperfine splittings with moderate uncertainties that are comparable to the recent lattice computations. It provides yet another evidence that perturbative QCD is compatible with the experimental data within estimated perturbative uncertainties [15–17]. Uncertainties of our
predictions for the bottomonium hyperfine splittings are much smaller than those for the charmonium.

The input parameters of our predictions are the quark $\overline{MS}$ masses and the strong coupling constant, apart from the scale that is varied within a reasonable range as part of the error analysis. In addition, our predictions are dependent on the specific prescriptions to define $E_{\text{imp}}(r)$ or on the specific organisation of our perturbative series. Nonetheless, our predictions together with the estimated uncertainties lie within the frame of perturbative QCD, hence, our formalism can be used for testing the validity of perturbative QCD in comparison with the experimental data. In this sense, the freedom we have in performing an analysis based on perturbative QCD is rather restricted: either we may find a more sophisticated prescription and reduce theoretical errors, or choose a poorer prescription and increase errors, other than changing the values of the aforementioned input parameters; we cannot incorporate any contributions which lie outside of perturbative QCD. This is in contrast with the conventional phenomenological models, which typically have much more input parameters; they can be adjusted so as to reproduce experimental data, without affecting uncertainties of theoretical predictions. Thus, we consider it quite non-trivial that the experimental data are reproduced with respect to moderate theoretical uncertainties, even though there appears to be some arbitrariness in defining our formalism.

Although our formalism predicts the complete spectrum, in this article we concentrated on the level splittings that have smaller theoretical uncertainties than the levels themselves. We have previously shown that our formalism also reproduces the overall bottomonium spectrum (as far as it is measured) well [17]. The same is true for charmonium, although theoretical uncertainties are larger in this case [27].

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When the manuscript for this paper was prepared, only the (inconsistent) Crystal Ball [19] and Belle [20] measurements for the $\eta_c(2S)$ mass were available, so both of them were quoted in Table 1. Very recently, several more new measurements have appeared that support the Belle value: BaBar measures $3630.8 \pm 3.4 \pm 1.0$ MeV [28] (an earlier analysis resulted in $3632.2 \pm 5.0 \pm 1.8$ MeV [29]), CLEO II gives $3642.7 \pm 4.1 \pm 4.0$ MeV (CLEO III prelim.: $3642.5 \pm 3.6 \pm? MeV$) [30] and a different Belle analysis yields $3630 \pm 8$ MeV [31]. The $\psi(2S) - \eta_c(2S)$ splitting calculated from a naive average of the central values of all measurements except Crystal Ball is 47 MeV, in excellent agreement with our results.
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