

Calculation of the quarkonium spectrum and m_b, m_c to order α_s^4

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We include two loop, relativistic one loop and second order relativistic tree level corrections, plus leading nonperturbative contributions, to obtain a calculation of the lower states in the heavy quarkonium spectrum correct up to, and including, $O(\alpha_s^4)$ and leading Λ^4/m^4 terms. This allows us, in particular, to obtain a model-independent determination of the pole masses of the b, c quarks, $m_b = 5015_{-70}^{+110}$ MeV, $m_c = 1884_{-133}^{+222}$ MeV, to which correspond the $\overline{\text{MS}}$ masses $\bar{m}_b(\bar{m}_b^2) = 4453_{-32}^{+50}$ MeV, $\bar{m}_c(\bar{m}_c^2) = 1547_{-102}^{+169}$ MeV. The decay $\Gamma(Y \rightarrow e^+e^-)$ is found to be in agreement with experiment, $\Gamma(Y \rightarrow e^+e^-) = 1.135_{-0.29}^{+0.27}$ keV (expt. = 1.320 ± 0.04 keV), and the hyperfine splitting is predicted to be $M(Y) - M(\eta) = 48.5_{-12.2}^{+15.7}$ MeV. [S0556-2821(98)06517-5]

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I. INTRODUCTION

In recent years it has become possible to perform rigorous QCD analyses of heavy quarkonium systems, and this due to two reasons. First, radiative corrections have been calculated to increasing order of accuracy. The one loop corrections to the nonrelativistic (NR) spin-independent (SI) potential were calculated already in 1980 [1]. This was extended in Refs. [2, 3] to the spin-dependent corrections and in Ref. [4] by including the velocity corrections to the SI part. Finally, the two loop nonrelativistic, spin-independent corrections to the potential have been evaluated recently [5].

Second, Leutwyler [6] and Voloshin [6] (see also Ref. [7]) have shown how to take into account, to leading order, nonperturbative (NP) effects, associated with the nonzero value of various condensates, of which the leading contribution is that of the gluon condensate $\langle \alpha_s G^2 \rangle$. This has been implemented, together with the potential obtained with radiative corrections to one loop, in Refs. [4, 8] where a study of bound states $\bar{b}b$ with $nl=10, 20, 21$ and $\bar{c}c$ states with $nl=10$ was given.¹ The analysis was extended in Refs. [9, 7] with the inclusion of size effects and higher condensates.

The overall conclusion of these analyses is that pure QCD, without recourse to introducing phenomenological interactions, produces a good description with manageable errors of the $\bar{b}b$ ground state and, to a lesser extent, of the splitting $M(Y) - M(\eta_b)$ and the decay $Y \rightarrow e^+e^-$. The description of the ground state of $\bar{c}c$ and of the excited states $n=2, l=0, 1$ of $\bar{b}b$ was shown to be even less reliable: the corrections are large, in some cases larger than the nominally leading terms. Still, it was possible, by using the renormalization point μ as a free parameter, to get a fairly accurate description of all $n=2$ states including tensor and LS splittings [8].

In the present paper we extend this analysis by including the two loop corrections to the SI, NR potential recently calculated [5], adding also velocity corrections to certain one loop pieces to get a calculation accurate up to, and including, $O(\alpha_s^4)$ corrections. By taking into account the leading nonperturbative terms, we also include in the analysis corrections of order Λ^4/m^4 . If we invert the calculations, we can deduce quark masses from the masses of the $Y, J/\psi$ particles. We then find, for the pole masses,

$$\begin{aligned} m_b &= 5015_{-70}^{+110} \text{ MeV}, \\ m_c &= 1884_{-133}^{+222} \text{ MeV}, \end{aligned} \quad (1.1a)$$

to which correspond the modified minimal subtraction scheme ($\overline{\text{MS}}$) masses

$$\begin{aligned} \bar{m}_b(\bar{m}_b^2) &= 4453_{-32}^{+50} \text{ MeV}, \\ \bar{m}_c(\bar{m}_c^2) &= 1547_{-102}^{+169} \text{ MeV}. \end{aligned} \quad (1.1b)$$

The error includes the estimated theoretical error of the calculation: see the text below. Note that Eqs. (1.1) are very precise, in the sense that they are correct to order α_s^4 and leading $O(\Lambda^4/m^4)$ nonperturbative effects. This is to be compared with estimates based on sum rules [10], which are only accurate to order α_s^2 , or previous bound state calculations [4], accurate only to third order in α_s . Nevertheless, it is true that the two loop corrections are large: their size is the only important weak point of the present calculation. We discuss this in some detail in Sec. V.

The decay $\Gamma(Y \rightarrow e^+e^-)$ is also given in agreement with experiment, within errors:

$$\begin{aligned} \Gamma(Y \rightarrow e^+e^-) &= 1.135_{-0.29}^{+0.27} \text{ keV} \\ &(\text{expt.} = 1.320 \pm 0.04 \text{ keV}). \end{aligned}$$

The hyperfine splitting is predicted to be

$$M(Y) - M(\eta) = 48.5_{-12.2}^{+15.7} \text{ MeV}.$$

¹Throughout this paper n and l will denote the principal quantum number and the angular momentum of bound states, respectively.

For higher states ($nl=20,21$) the errors are much larger, but within these, one has compatibility with experiment (cf. Sec. IV C).

II. EFFECTIVE POTENTIAL

We follow the method of effective potentials of Gupta *et al.* [3] and the renormalization scheme of Ref. [4]. The Hamiltonian for quarkonium may then be split in the following form:

$$H = H^{(0)} + H_1 \quad (2.1a)$$

where $H^{(0)}$ is

$$H^{(0)} = 2m + \frac{-1}{m} \Delta - \frac{C_F \tilde{\alpha}_s(\mu^2)}{r},$$

$$\tilde{\alpha}_s(\mu^2) = \alpha_s(\mu^2) \left\{ 1 + \left(a_1 + \frac{\gamma_E \beta_0}{2} \right) \frac{\alpha_s(\mu^2)}{\pi} \right.$$

$$\left. + \left[\gamma_E \left(a_1 \beta_0 + \frac{\beta_1}{8} \right) + \left(\frac{\pi^2}{12} + \gamma_E^2 \right) \frac{\beta_0^2}{4} + b_1 \right] \frac{\alpha_s^2}{\pi^2} \right\}$$
(2.1b)

and can (and will) be solved exactly. H_1 may be written as

$$H_1 = V_{\text{tree}} + V_1^{(L)} + V_2^{(L)} + V^{(LL)} + V_{\text{s,rel}} + V_{\text{spin}}, \quad (2.1c)$$

and

$$V_{\text{tree}} = \frac{-1}{4m^3} \Delta^2 + \frac{C_F \alpha_s}{m^2 r} \Delta,$$

$$V_1^{(L)} = \frac{-C_F \beta_0 \alpha_s(\mu^2)^2 \log r \mu}{2\pi r},$$

$$V_2^{(L)} = \frac{-C_F \alpha_s^3}{\pi^2} \left(a_1 \beta_0 + \frac{\beta_1}{8} + \frac{\gamma_E \beta_0^2}{2} \right) \frac{\log r \mu}{r}$$

$$\equiv \frac{-C_F c_2^{(L)} \alpha_s^3 \log r \mu}{\pi^2 r},$$

$$V^{(LL)} = \frac{-C_F \beta_0^2 \alpha_s^3 \log^2 r \mu}{4\pi^2 r},$$

$$V_{\text{s,rel}} = \frac{C_F a_2 \alpha_s^2}{2m r^2},$$

$$V_{\text{spin}} = \frac{4\pi C_F \alpha_s}{3m^2} s(s+1) \delta(\mathbf{r}). \quad (2.1d)$$

Here the running coupling constant has to be taken to three loops. For the values of the constants entering the above formulas (cf. the Appendix), a_1 was calculated in Ref. [1], a_2 in Ref. [4], and b_1 in Ref. [5]. The other terms in Eq. (2.1d) can be obtained by use of the renormalization group

(see, e.g., Ref. [4]) or are well-known tree level relativistic corrections (including kinetic energy corrections).

A few words are due on Eqs. (2.1). First of all, they only take into account the *perturbative* part of the calculation; NP effects will be incorporated later. Second, it should be noted that H_1 contains a velocity-dependent one loop piece $V_{\text{s,rel}}$. This is because the average velocity in a Coulombic potential is $\langle |v| \rangle \sim \alpha_s$: hence, a calculation correct to order α_s^4 requires tree level $O(v^2)$ and one loop $O(|v|)$ contributions. All these terms in H_1 may be treated as perturbations to first order, *except* $V_1^{(L)}$. For this, the second order perturbative contribution is required as this also produces a correction of order α_s^4 .

A last comment concerns the renormalization scheme. We have followed Ref. [4] in renormalizing α_s in the $\overline{\text{MS}}$ scheme, but the mass m that appears in Eqs. (2.1) is the two loop pole mass. That is to say, it is defined by the equation

$$S_2^{-1}(\not{p}=m, m) = 0, \quad (2.2)$$

where $S_2(\not{p}, m)$ is the quark propagator to two loops. One can relate m to the $\overline{\text{MS}}$ parameter, also to two loop accuracy, using the results of Ref. [11]:

$$\bar{m}(\bar{m}^2) = m \left\{ 1 + \frac{C_F \alpha_s(m^2)}{\pi} + (K - 2C_F) \left(\frac{\alpha_s}{\pi} \right)^2 \right\}^{-1},$$

$$K(n_f=4) \simeq 13.4, \quad K(n_f=3) \simeq 14.0. \quad (2.3)$$

III. ENERGY SHIFTS

A. Order α_s^4 , Λ^4/m^4

Taking into account the expression for the Hamiltonian, Eq. (2.1), we can write

$$E_{nl} = 2m - m \frac{C_F^2 \tilde{\alpha}_s^2}{4n^2} + \sum_V \delta_V^{(1)} E_{nl} + \delta_{V_1}^{(2)} E_{nl} + \delta_{\text{NP}} E_{nl}. \quad (3.1)$$

Here the $\delta_V^{(1)} E_{nl}$ may be easily evaluated with the formulas in the Appendix to Ref. [4]. We define generally the analogue of the Bohr radius,

$$a(\mu^2) = \frac{2}{m C_F \tilde{\alpha}_s(\mu^2)},$$

and, then,

$$\delta_{V_{\text{tree}}}^{(1)} E_{nl} = - \frac{2}{n^3 m^3 a^4} \left[\frac{1}{2l+1} - \frac{3}{8n} \right] + \frac{C_F \alpha_s}{m^2} \frac{2l+1-4n}{n^4 (2l+1) a^3}, \quad (3.2a)$$

$$\delta_{V_1}^{(1)} E_{nl} = - \frac{\beta_0 C_F \alpha_s^2(\mu^2)}{2\pi n^2 a} \left[\log \frac{n a \mu}{2} + \psi(n+l+1) \right], \quad (3.2b)$$

$$\delta_{V_2^{(L)}}^{(1)} E_{nl} = -\frac{C_{FC_2^{(L)}} \alpha_s^3}{\pi^2 n^2 a} \left[\log \frac{na\mu}{2} + \psi(n+l+1) \right], \quad (3.2c)$$

$$\delta_{V_{(LL)}}^{(1)} E_{nl} = -\frac{C_F \beta_0^2 \alpha_s^3}{4 \pi^2 n^2 a} \left\{ \log^2 \frac{na\mu}{2} + 2\psi(n+l+1) \log \frac{na\mu}{2} \right. \\ \left. + \psi(n+l+1)^2 + \psi'(n+l+1) + \theta(n-l-2) \right. \\ \left. \times \frac{2\Gamma(n-l)}{\Gamma(n+l+1)} \sum_{j=0}^{n-l-2} \frac{\Gamma(2l+2+j)}{j!(n-l-j-1)^2} \right\}, \quad (3.2d)$$

$$\delta_{V_{s,rel}}^{(1)} E_{nl} = \frac{C_{FA_2} \alpha_s^2}{m} \frac{1}{n^3 (2l+1) a^2}. \quad (3.2e)$$

We recall that constants are collected in the Appendix. For the vector states ($Y, Y', Y''; J/\psi, \psi', \dots$) one has to add the hyperfine shift, at the tree level,

$$\delta_{V_{spin}}^{(1)} E_{nl} = \delta_{s1} \delta_{l0} \frac{8C_F \alpha_s}{3n^3 m^2 a^3}. \quad (3.2f)$$

The calculation of the second order contribution of $V_1^{(L)}$, $\delta_{V_1^{(L)}}^{(2)} E_{nl}$, is nontrivial and may be found in the Appendix.

We define

$$\delta_{V_1^{(L)}}^{(2)} E_{nl} = -m \frac{C_F^2 \beta_0^2 \alpha_s^4}{4n^2 \pi^2} \left\{ N_0^{(n,l)} + N_1^{(n,l)} \log \frac{na\mu}{2} \right. \\ \left. + \frac{1}{4} \log^2 \frac{na\mu}{2} \right\}, \quad (3.3a)$$

and then one has, for the lowest states,

$$N_1^{(1,0)} = -\frac{\gamma_E}{2} \approx -0.288608,$$

$$N_1^{(2,0)} = \frac{1-2\gamma_E}{4} \approx -0.0386078,$$

$$N_1^{(2,1)} = \frac{5-6\gamma_E}{12} \approx 0.128059,$$

$$N_0^{(1,0)} = \frac{3+3\gamma_E^2-\pi^2+6\zeta(3)}{12} \approx 0.111856,$$

$$N_0^{(2,0)} = -\frac{5}{16} - \frac{\gamma_E}{4} + \frac{\gamma_E^2}{4} - \frac{\pi^2}{12} + \zeta(3) \approx 0.00608043,$$

$$N_0^{(2,1)} = -\frac{865}{432} - \frac{5\gamma_E}{12} + \frac{\gamma_E^2}{4} - \frac{11\pi^2}{36} + \zeta(3) \approx 0.0314472. \quad (3.3b)$$

In addition to this one has to consider the NP energy splittings. The dominant ones are associated with the gluon condensate and are [6]

$$\delta_{NP} E_{nl} = m \epsilon_{nl} n^2 \pi \langle \alpha_s G^2 \rangle \left(\frac{na}{2} \right)^4 = m \frac{\epsilon_{nl} n^6 \pi \langle \alpha_s G^2 \rangle}{(m C_F \tilde{\alpha}_s)^4},$$

$$\epsilon_{10} = \frac{1872}{1275}, \quad \epsilon_{20} = \frac{2102}{1326}, \quad \epsilon_{21} = \frac{9929}{9945}. \quad (3.4)$$

Because $\langle \alpha_s G^2 \rangle \sim \Lambda^4$, this is of order $(\Lambda/m)^4$, albeit with large coefficients: for all terms we have a fourth power of α_s in the denominator, and for $n > 1$ the n^6 in the numerator of Eq. (3.4) grows very quickly out of hand. In fact, it is the size of this term that limits the range of validity of our type of *ab initio* calculation.

B. Higher corrections

In addition to the corrections reported in the previous subsection, there are a few pieces of the higher order corrections that are known. First of all, we have the relativistic $O(v^2)$ corrections to the one loop potential [4]. These produce corrections of higher order, α_s^5 , but they are logically independent of the *three loop* ones that would produce terms of the same order, but, presumably, smaller because of the extra $1/\pi^2$ characteristic of radiative corrections. These corrections may be incorporated and then can be considered to give an indication of the error committed in neglecting higher order *perturbative* corrections. They produce, for the ground state, the energy shift (Ref. [4], typographical errors corrected in Ref. [8])

$$\delta_{1\text{loop},v^2}^{(1)} E_{10} = A_5 + A_S,$$

$$A_5 = 2m \left\{ -\frac{3C_F^4 \beta_0}{32\pi} \left[\log \frac{\mu}{m C_F \tilde{\alpha}_s} - \frac{1}{3} - \gamma_E \right] \right. \\ \left. - \frac{3C_F^4}{16\pi} \left(a_1 + \frac{\beta_0 \gamma_E}{2} \right) - \frac{C_F^4 a_3}{16\pi} \left[\log \frac{1}{C_F \tilde{\alpha}_s} - 1 \right] \right. \\ \left. + \frac{C_F^4 [a_5 - (\frac{5}{6} + \log \tilde{n}) a_4]}{16\pi} \right\} \alpha_s^2 \tilde{\alpha}_s^3, \\ A_S = 2m \delta_{s1} \frac{C_F^4}{6\pi} \left\{ \frac{\beta_0}{2} \left(\log \frac{na\mu}{2} - \sum_1^n \frac{1}{k} - \frac{n-1}{2n} \right) \right. \\ \left. - \frac{21}{4} \left(\log \frac{n}{C_F \tilde{\alpha}_s} - \sum_1^n \frac{1}{k} - \frac{n-1}{2n} \right) + B \right\} \alpha_s^2 \tilde{\alpha}_s^3. \quad (3.5)$$

Next, we have higher order NP corrections. These include finite size corrections, estimated in Ref. [7], and contributions of higher dimensional operators, some of which were evaluated in Ref. [9]. The last produce the shifts

$$\delta_{NP,higher} = \frac{-1}{m^5 (C_F \tilde{\alpha}_s)^8} h(n,l) O_6,$$

TABLE I. Determinations of the b quark mass with increasing accuracy.

	$O(\alpha_s^2)$	$O(\alpha_s^3)$	One loop+rel. ^a	$O(\alpha_s^4)$
μ^2 (GeV ²)	3.233	4.940	≈ 2.5	7.019
m_b (GeV)	4.752	4.858	4.939 ^a	$5.015_{-0.064}^{+0.101}(\Lambda) \mp 0.005(\langle\alpha_s G^2\rangle)_{\pm 0.041}^{-0.027}$ (vary μ^2 by 25%)
$\bar{m}_b(\bar{m}_b^2) =$	4.209	4.307	4.382 ^a	$4.453_{-0.015}^{+0.029}(\Lambda) \mp 0.004(\langle\alpha_s G^2\rangle)_{\pm 0.038}^{-0.025}$ (vary μ^2 by 25%)

^aThis value is taken from Ref. [4], extrapolated to $\Lambda = 0.23$ GeV, $\langle\alpha_s G^2\rangle = 0.06$ GeV⁴.

$$h(1,0) = \frac{141\,912\,051\,712}{844\,421\,875},$$

$$h(2,0) = \frac{484\,859\,657\,191\,424}{2\,040\,039\,729},$$

$$h(2,1) = \frac{102\,150\,951\,135\,870\,976}{765\,014\,898\,375},$$

$$O_6(\mu) = \frac{1}{108} \left\{ \frac{2^6}{3} \pi^2 \alpha_s(\mu) \kappa + \frac{3}{4} \langle G^3 \rangle \right\},$$

$$\kappa = \alpha_s \langle 0 | \bar{q}q | 0 \rangle^2, \quad (3.6)$$

and may be used to estimate the size of the higher order NP contributions. For the quark condensate the vacuum saturation approximation is assumed, and the value of κ is taken from Ref. [12]. For $\langle G^3 \rangle$ one takes the value 0.065 GeV⁶. Anyway, these quantities are poorly known.

It is important to realize that both Eqs. (3.5) and (3.6) should be taken as *indications*. With respect to the first, there is no guarantee that the coefficient of the three loop correction is not so large that it offsets the factors of $1/\pi$; indeed, this already happens to two loops where the coefficient is large, $b_1 \approx 24$. With respect to Eqs. (3.6) and apart from the fact that it does not include all the higher dimensional operators (those associated with size corrections are neglected²), it is clear that one cannot consider rigorously a contribution $O(\Lambda^6/m^6)$ as long as the radiative corrections to the $O(\Lambda^4/m^4)$ terms are not known. Nevertheless, we consider Eqs. (3.5) and (3.6) as very useful for estimating the theoretical uncertainties of our calculation.

IV. NUMERICAL RESULTS

Using the formulas deduced above, one can evaluate the spectrum of heavy quarkonium systems. In principle, one should take m , Λ , $\langle\alpha_s G^2\rangle$ from other sources and predict the masses of the quarkonium states. In practice, it is better to use the known masses of the lowest states (Y and J/ψ) to *evaluate* the quark masses. The reason is that this produces

²The reason for doing so is that, at least nominally, the contribution of operators associated with the size, $\langle[\partial G(0)]^2\rangle$, is of higher order in α_s than the ones considered in Eqs. (3.6). See Ref. [9] for details.

the more precise evaluation available at present of these parameters, especially in the case of the b quark. The other parameters we take from independent sources. For the QCD parameter Λ , we take, throughout this section,

$$\Lambda(n_f=4, \text{ three loops}) = 0.23_{-0.05}^{+0.08} \text{ GeV}$$

$$[\alpha_s(M_Z^2) \approx 0.114_{-0.004}^{+0.006}], \quad (4.1a)$$

and for the gluon condensate, very poorly known,

$$\langle\alpha_s G^2\rangle = 0.06 \pm 0.02 \text{ GeV}^4. \quad (4.1b)$$

Note that this value of $\alpha_s(M_Z^2)$ is slightly smaller than, though compatible with, the world average $\alpha_s(M_Z^2) = 0.118$. We have preferred the value (4.1b), which is obtained averaging measurements performed at *spacelike* momenta; see the recent review of Bethke [13].

Another matter to be discussed is the choice of the renormalization point μ . As our equations (3.2), (3.3) show, a *natural* value for this parameter is

$$\mu = \frac{2}{na}, \quad (4.1c)$$

for states with the principal quantum number n , and this will be our choice. For states with $n=1$ the results of the calculation will turn out to depend little on the value of μ , provided it is reasonably close to Eq. (4.1c). Higher states are another matter; we will discuss our choices when we consider them.

A. 10 state of $\bar{b}b$ and the mass m_b

As stated, we select, for the Y state, $\mu = 2/a$. We then use Eqs. (3.1)–(3.4) to obtain the values of the b quark mass. To make apparent the contribution of the higher corrections, we have performed calculations taking into account only $O(\alpha_s^2)$, $O(\alpha_s^3)$, $O(\alpha_s^3) + |v| \times$ one loop terms and, finally, the full $O(\alpha_s^4)$ evaluation. The results are reported in Table I,³ where the errors correspond to the errors in Eqs. (4.1a), (4.1b).

In the estimate of the errors, the condition $\mu = 2/a$ is

³We have arranged in Table I the results in terms of powers of α_s ; we could have arranged them in increasing number of loops. Cf. Sec. V for this.

maintained satisfied when varying Λ , while for the error due to the variation of μ the other parameters are kept fixed (i.e., one then no longer has $\mu=2/a$). The dependence of m_b on μ should be taken as an indication of the theoretical uncertainty

of our calculation. To estimate other theoretical errors in our evaluation, we proceed as follows. We either calculate m_b including the full $O(v^2)$ corrections to one loop, Eqs. (3.5). Then we get

$$\text{(one loop+rel.)+(two loop, NR): } t=7.009, \quad m_b=5.010, \quad \bar{m}_b(\bar{m}_b^2)=4.448, \quad (4.2a)$$

or we may include the contribution of higher dimensional NP effects, as in Eqs. (3.6). Then,

$$\text{with higher NP effects: } m_b=5.018, \quad \bar{m}_b(\bar{m}_b^2)=4.455. \quad (4.2b)$$

We consider that the best result is that of $O(\alpha_s^4)$ reported in Table I and take the difference with the quantities given in Eqs. (4.2) as a further estimation of the theoretical error of the calculation. In this way we get our best estimate

$$m_b=5.015_{-0.064}^{+0.101}(\Lambda) \mp 0.005(\langle \alpha_s G^2 \rangle)_{+0.041}^{-0.027} \text{ (vary } \mu^2 \text{ by 25\%)} \pm 0.006 \text{ (other th. uncertainty),}$$

$$\bar{m}_b(\bar{m}_b^2)=4.453_{-0.016}^{+0.029}(\Lambda) \mp 0.004(\langle \alpha_s G^2 \rangle)_{+0.038}^{-0.025} \text{ (vary } \mu^2 \text{ by 25\%)} \pm 0.005 \text{ (other th. uncertainty).} \quad (4.3)$$

The values of $\alpha_s(\mu^2)$, $\tilde{\alpha}_s(\mu^2)$ corresponding to $\mu^2=7.019 \text{ GeV}^2$ are

$$\alpha_s(\mu^2)=0.24, \quad \tilde{\alpha}_s(\mu^2)=0.40.$$

The piece denoted by the expression ‘‘other th. uncertainty’’ in Eqs. (4.3), which refers to the error coming from higher dimensional operators and higher order perturbative terms, Eqs. (4.2), is comfortably smaller than the errors due to the uncertainty on Λ , $\langle \alpha_s G^2 \rangle$. We will henceforth omit these errors, so as not to double count them, and consider that the theoretical error is only that due to varying μ^2 by 25%. If we now compose all the errors quadratically, then we obtain the estimate reported in the Introduction, Eqs. (1.1).

B. $M(Y)-M(\eta_b)$: The decay $Y \rightarrow e^+e^-$

The evaluation of Refs. [4,8] for the hyperfine splitting and the decay of the Y into e^+e^- does not change, except that the favored values of Λ , $\langle \alpha_s G^2 \rangle$, and m_b are now somewhat different. This improves slightly the agreement with experiment for the decay rate. The expressions are

$$M(V)-M(\eta)$$

$$=m \frac{C_F^4 \alpha_s(\mu^2) \tilde{\alpha}_s(\mu^2)^3}{3} [1 + \delta_{\text{wf}} + \delta_{\text{NP}}]^2$$

$$\times \left\{ 1 + \left[\frac{\beta_0}{2} \left(\log \frac{a\mu}{2} - 1 \right) + \frac{21}{4} (\log C_F \tilde{\alpha}_s + 1) + B \right] \right.$$

$$\left. \times \frac{\alpha_s}{\pi} + \frac{1161}{8704} \frac{\pi \langle \alpha_s G^2 \rangle}{m^4 \tilde{\alpha}_s^6} \right\}, \quad (4.4a)$$

$$\Gamma(Y \rightarrow e^+e^-) = \Gamma^{(0)} [1 + \delta_{\text{wf}} + \delta_{\text{NP}}]^2 (1 + \delta_{\text{rad}}),$$

$$\Gamma^{(0)} = 2 \left[\frac{Q_b \alpha_{\text{QED}}}{M(Y)} \right]^2 [m C_F \tilde{\alpha}_s(\mu^2)]^3,$$

$$\delta_{\text{rad}} = - \frac{4 C_F \alpha_s}{\pi},$$

$$\delta_{\text{wf}} = \frac{3\beta_0}{4} \left(\log \frac{a\mu}{2} - \gamma_E \right) \frac{\alpha_s}{\pi},$$

$$\delta_{\text{NP}} = \frac{1}{2} \left[\frac{270459}{108800} + \frac{1838781}{2890000} \right] \frac{\pi \langle \alpha_s G^2 \rangle}{m^4 \tilde{\alpha}_s^6}. \quad (4.4b)$$

The corrections here are fairly large, particularly the radiative correction [14] δ_{rad} . Because of this, the calculation is less reliable than what one would have expected. With the values of m_b found in Eqs. (4.3), one has the numerical results

$$M(Y)-M(\eta) = 48.4_{-4.8}^{+13.1}(\Lambda)_{-4.6}^{+4.9}(\langle \alpha_s G^2 \rangle)_{-10.2}^{+7.2}$$

$$(\mu^2 = 7.019 \pm 25\%) \quad (4.5)$$

and

$$\Gamma(Y \rightarrow e^+e^-) = 1.135_{-0.02}^{+0.15}(\Lambda) \pm 0.11(\langle \alpha_s G^2 \rangle)_{-0.27}^{+0.19}$$

$$(\mu^2 = 7.019 \pm 25\%). \quad (4.6)$$

Note that, when varying Λ , $\langle \alpha_s G^2 \rangle$, we have varied m_b according to Eqs. (4.3), but we have *not* varied m_b when varying μ .

Higher order NP corrections due to the higher dimensional operators introduced in Eqs. (3.6) are also known for the decay rate (see Ref. [9]). They read

$$\delta_{\text{NNP}} = \frac{w(n)}{2m^6(C_F\bar{\alpha})^{10}} O_6,$$

$$w(1) = -\frac{1\ 670\ 626\ 488\ 940\ 208\ 128}{485\ 563\ 688\ 671\ 875}.$$

Size corrections, however, are not known now. δ_{NNP} would produce a shift in the decay rate of ~ 0.11 keV, smaller than the contribution of $\langle\alpha_s G^2\rangle$ or the uncertainty caused by, e.g., varying μ as in Eqs. (4.3). We do *not* include δ_{NNP} either in the evaluation or the error estimate.

The result for the decay is in reasonable agreement with experiment:

$$\Gamma_{\text{expt}}(Y \rightarrow e^+ e^-) = 1.320 \pm 0.04 \text{ keV}.$$

Composing the errors, we obtain the figures quoted in the Introduction, Eqs. (1.1a), (1.1b).

C. Higher states ($n=2$) of $\bar{b}b$

The masses of the states with $n=2$ will be next determined. As is clear from the expressions (3.2), (3.3) the natural choice of scale is now $\mu=1/a$, which gives $\mu^2=3.05 \text{ GeV}^2$. If we take this, adding or subtracting 25% to estimate the dependence of the calculation on the choice of scale, then we obtain the results

$$M(20, \text{th}) - M(20, \text{expt}) = 293_{-299}^{+286} \text{ MeV}$$

$$(\mu^2 = 3.048 \pm 25\%),$$

$$M(21, \text{th}) - M(21, \text{expt}) = 174_{-203}^{+191} \text{ MeV}$$

$$(\mu^2 = 3.048 \pm 25\%). \quad (4.7)$$

We only present the errors that follow from variation of the scale μ^2 by 25%; slightly smaller ones are produced by the errors of Λ , $\langle\alpha_s G^2\rangle$. We do not make explicit this: because of the size of the errors in Eq. (4.7), there is no point in going for a more detailed error analysis.

Although they have decreased from the one loop evaluations (e.g., Ref. [4]), the errors are still fairly large here; within them, there is compatibility between theory and experiment. Agreement to a few MeV for both states is obtained if choosing $\mu^2=0.75/a \approx 2.3 \text{ GeV}^2$ or keeping $\mu=1/a$ and taking $\langle\alpha_s G^2\rangle=0.036 \text{ GeV}^4$: unlike for the states with $n=1$, we have now strong dependence of the results on the parameters of the calculation. This is due to the *large* size of the corrections, perturbative and (especially) nonperturbative. This last is made more apparent when considering contributions of higher dimensional operators [9], which get completely out of hand for $nl=20$ and are very large for $nl=21$. In this context, it is satisfactory to realize that it is for this last state (21) for which agreement with experiment is best and theoretical errors smaller.

We will not discuss here the spin and tensor splittings among the states with $nl=21$. The inclusion of three loop corrections to the potential only affects their calculation in that the preferred value for m_b will be different now, which is a minute effect compared with the uncertainties of the calculation: one should realize [8] that, while the NP corrections to the energy levels with principal quantum number n contain a coefficient $n^6/\bar{\alpha}_s^4$, wave functions at the origin get a factor $\sim n^8/\bar{\alpha}_s^6$. This of course is what makes the calculation of $M(Y) - M(\eta_b)$ and the decay $Y \rightarrow e^+ e^-$ much less reliable than that of $M(Y)$ (or, equivalently, m_b) and what makes the evaluation of tensor and spin splittings with $n=2$ somewhat marginal. All one can do here is *fit* μ to the data; this is the procedure followed in Ref. [8], and we have nothing new to report on this.

D. 10 state of $\bar{c}c$ and the mass m_c

The value of the parameter Λ used now, corresponding to that in Eq. (4.1a), is

$$\Lambda(n_f=3, \text{ three loops}) = 0.30_{-0.05}^{+0.09} \text{ GeV}.$$

The values for the c quark mass, deduced from the J/ψ mass, are, then,

$$O(\alpha_s^4): \quad t=2.623, \quad m_c=1.884, \quad \bar{m}_c(\bar{m}_c^2)=1.547;$$

$$(\text{one loop+rel.})+(\text{two loop, NR}): \quad t=2.611, \quad m_c=1.875, \quad \bar{m}_c(\bar{m}_c^2)=1.539;$$

$$\text{with higher NP effects:} \quad t=2.634, \quad m_c=1.891, \quad \bar{m}_c(\bar{m}_c^2)=1.554. \quad (4.8)$$

Including errors we obtain the best estimate, analogous to that in Eqs. (4.3) for the b quark:

$$m_c = 1.884_{-0.092}^{+0.157}(\Lambda) \mp 0.012(\langle\alpha_s G^2\rangle)_{+0.156}^{-0.096}(\text{varying } \mu^2 \text{ by } 25\%) \pm 0.011 \text{ (th. uncertainty),}$$

$$\bar{m}_c(\bar{m}_c^2) = 1.547_{-0.049}^{+0.086}(\Lambda) \mp 0.011(\langle\alpha_s G^2\rangle)_{+0.145}^{-0.089}(\text{varying } \mu^2 \text{ by } 25\%) \pm 0.010 \text{ (th. uncertainty).} \quad (4.9)$$

As is obvious from these equations, the errors are now much larger than for the b quark case, but our determination of m_c still competes in accuracy with those based on QCD sum rules.

V. DISCUSSION

The calculations of this paper are rather straightforward, but there are a few points that merit further discussion. First of all, our values for the quark masses are somewhat larger than existing estimates based on sum rules, for the MS masses, of 100–300 MeV; cf. Ref. [10]. In our opinion this is due to the influence of the terms of order α_s^3 , α_s^4 which we take into account, but which the sum rule evaluations, which stop at $O(\alpha_s^2)$, do not.

Second, and from Table I, it may appear that the series is *diverging*: from the $O(\alpha_s^2)$ to the $O(\alpha_s^3)$ evaluation, m_b increases by 106 MeV, but from the last to the $O(\alpha_s^4)$, the increase is of 157. Actually, convergence is not too bad, although one is likely at the edge of the region of convergence for the series. The increase between $O(\alpha_s^3)$ and $O(\alpha_s^4)$ is due to two *independent* factors: inclusion of the two loop corrections to the potential, responsible for 46 MeV, and the relativistic corrections. Of these, 64 MeV are for tree level corrections and 40 MeV are for the mixed one loop velocity correction. Each of the effects is small. Thus, if we included velocity corrections at every loop, the variation from zero to one to two loops would be *diminishing*. This is apparent if we compare the value obtained in Ref. [4] (corrected for the increased values of Λ , $\langle\alpha_s G^2\rangle$ we are using now) with our results, with a variation of only 60 MeV. One can see this more clearly if we arrange the calculation in increasing number of loops including, at every step, the pertinent relativistic corrections⁴ or including all loop corrections, but in increasing order of the velocity corrections:

$$m_b = \begin{cases} \text{tree level incl. rel. correct's.:} & 4.758; \\ \text{one loop incl. rel. correct's.:} & 4.893; \\ \text{full calculation:} & 5.015; \end{cases}$$

$$m_b = \begin{cases} \text{static, two loop:} & 4.962; \\ \text{full calc.:} & 5.015. \end{cases}$$

Finally, we remark on the reasonable stability we now have against variation of the renormalization scale μ . This stability of the results against changes of μ is made apparent by the fact that even multiplying or dividing the central value $\mu^2=7.019$ by a factor of 2 only alters the central value of $m_b=5.015$ GeV by 98 MeV. The stability is due mostly to the inclusion of two loop effects, but attention should also be paid to the stabilizing influence of the NP corrections. These corrections are larger for larger μ , exactly the opposite to

what happens to the perturbative corrections. One could even fix optimal values of μ as those where the combined perturbative-NP effects would show a minimal dependence on μ . This is essentially the procedure adopted in Ref. [4].

To finish this paper we devote a few words to the *error* estimates. As remarked at the end of Sec. IV A, we have, to get the main result, Eqs. (1.1), composed the errors due to variation of Λ , μ , and $\langle\alpha_s G^2\rangle$ as well as inclusion of estimated higher order terms as if they were *independent*—which they are not. Alternatively, we may keep all these quantities fixed at their central values, not include estimated higher orders, and estimate the errors by varying the renormalization point μ^2 by a factor of 2, $\mu^2=3.5\text{--}14$ GeV². For the b quark mass this would give

$$m_b = 5015_{-78}^{+119} \text{ MeV}, \quad \bar{m}_b(\bar{m}_b^2) = 4453_{-72}^{+110} \text{ MeV}. \quad (5.1)$$

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APPENDIX

Constants:

$$\beta_0 = 11 - \frac{2}{3}n_f, \quad \beta_1 = 102 - \frac{38}{3}n_f,$$

$$\beta_2 = \frac{2847}{2} - \frac{5033}{18}n_f + \frac{325}{54}n_f^2,$$

$$a_1 = \frac{31C_A - 20T_F n_f}{36} \simeq 1.47, \quad a_2 = \frac{C_F - 2C_A}{2} \simeq -2.33;$$

$$b_1 = \frac{1}{16} \left\{ \left[\frac{4343}{162} + 6\pi^2 - \frac{1}{4}\pi^4 + \frac{22}{3}\zeta(3) \right] C_A^2 \right.$$

$$\left. - \left[\frac{1798}{81} + \frac{56}{3}\zeta(3) \right] C_A T_F n_f \right.$$

$$\left. - \left[\frac{55}{3} - 16\zeta(3) \right] C_F T_F n_f + \frac{400}{81} T_F^2 n_f^2 \right\}$$

$$\simeq 24.30,$$

$$c_2^{(L)} = a_1 \beta_0 + \frac{1}{8} \beta_1 + \frac{1}{2} \gamma_E \beta_0^2,$$

$$a_3 = \frac{14C_F - 21C_A}{3}, \quad a_4 = \frac{-16C_F + 4C_A}{3},$$

$$a_5 = 2C_F + \frac{8C_A}{3} - \frac{64T_F}{15} + 4T_F \log 2,$$

$$B = \frac{3}{2}(1 - \log 2)T_F - \frac{5}{9}T_F n_f + \frac{11C_A - 9C_F}{18} \simeq 0.29.$$

⁴Nevertheless, it is true that the two loop correction is large: $b_1 \sim 24$, $b_1/\pi^2 \sim 2.5$, and $\alpha_s^2 b_1/\pi^2 \sim 0.14$, to be compared with $a_1/\pi \sim 0.5$, $\alpha_s a_1/\pi \sim 0.11$. As commented before, one is clearly near the limit of convergence of the perturbative series.

Second order contribution. We now calculate $\delta_{V^{(L)}}^{(2)} E_{nl}$. A simple and rather accurate approximation may be obtained

with use of the following trick. The second order shift given by a potential W may be written as

$$\delta_W^{(2)} E_{nl} = \langle nl | W | \delta^{(1)} R_{nl} \rangle,$$

where

$$|\delta^{(1)} R_{nl}\rangle = P_{nl} |R_{nl}^{(1)}\rangle;$$

P_{nl} is the projector orthogonal to the state nl and

$$|R_{nl}^{(1)}\rangle = |nl\rangle + \sum_{n' \neq n} \frac{1}{E_n - E_{n'}} |n'l\rangle \langle n'l | W | nl \rangle$$

is the wave function to first order. The trick is to use for this not the result of a Rayleigh-Schrödinger formula, but that obtained from a variational principle. For our case [cf. Ref. [4], Eqs. (79)–(81)],

$$R_{nl}^{(1)} = \frac{2}{n^2 b^{3/2}} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \left(\frac{2r}{nb} \right) e^{-r/nb} L_{n-l-1}^{2l+1}(2r/nb),$$

$$b^{-1} = a^{-1} \left[1 + \frac{\log(na\mu/2) + \psi(n+l+1) - 1}{2\pi} \beta_0 \alpha_s \right].$$

For the ground state, this gives, after a trivial calculation,

$$\delta_{V_1^{(L)}}^{(2)} E_{10} = -m \frac{\beta_0^2 C_F^2 \alpha_s^3 \tilde{\alpha}_s}{16\pi^2} \left[\log^2 \frac{a\mu}{2} - \gamma_E \right]^2.$$

This simple method gives correctly the coefficients of $\log a\mu$, $\log^2 a\mu$ and misses the constant term by $\sim 10\%$.

For the *exact* calculation one uses the representation of the Coulombic Green's function given, e.g., by Voloshin.⁵ We write

⁵An estimate neglecting the continuum contribution has been given in Ref. [15]. The approximation is not good, although since the quantity is small its effect in the evaluation of m_b was not important.

$$\delta_{V_1^{(L)}}^{(2)} E_{nl} = \sum_{k \neq n} \frac{|\langle n, l | V_1^{(L)} | k, l \rangle|^2}{E_n - E_k},$$

and the sum over k includes an integral over the continuous part of the spectrum. Instead of doing this computation directly, we have used the more general function

$$\begin{aligned} \sum_k \frac{|\langle n, l | V_1^{(L)} | k, l \rangle|^2}{E - E_k} &= \frac{|\langle n, l | V_1^{(L)} | n, l \rangle|^2}{E - E_n} \\ &+ \sum_{k \neq n} \frac{|\langle n, l | V_1^{(L)} | k, l \rangle|^2}{E - E_k} \\ &= \frac{A_{(-1)}}{E - E_n} + A_{(0)} + A_{(1)}(E - E_n) + \dots \end{aligned}$$

and then $\delta_{V_1^{(L)}}^{(2)} E_{nl} = A_{(0)}$. For the function defined above one uses the representation of the Coulombic Green's function given, e.g., by Voloshin in the second article in Ref. [6] [note that there is a misprint in formula (15) there, and $(s+l+1)!$ must be changed to $(s+2l+1)!$]. In this way we get for the different N_{nl} defined in Eq. (3.3) and for arbitrary quantum numbers,

$$N_1^{(n,l)} = \frac{\psi(1+l+n) - 1}{2},$$

$$N_0^{(n,l)} = \frac{1}{4} \psi(1+l+n) [\psi(1+l+n) - 2]$$

$$\begin{aligned} &+ \frac{n}{2} \left[\frac{(n-l-1)!}{(n+l)!} \sum_{s=0}^{n-l-2} \frac{(s+2l+1)!}{s!(s+l+1-n)^3} \right. \\ &+ \left. \frac{(n+l)!}{(n-l-1)!} \sum_{s=n-l}^{\infty} \frac{s!}{(s+2l+1)!(s+l+1-n)^3} \right]. \end{aligned}$$

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