Rigorous QCD evaluation of spectrum and other properties of heavy $q\bar{q}$ systems: Bottomonium with $n = 2$, $l = 0, 1$

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(Received 6 April 1994; revised manuscript received 9 September 1994)

We calculate the Lamb, fine, and hyperfine shifts in $b\bar{b}$ with $n = 2$, $l = 0, 1$. Radiative corrections as well as leading nonperturbative corrections (known to be due to the gluon condensate) are taken into account. Taking Λ and $\langle\alpha_s G^2\rangle$ from independent sources, we find agreement with experiment at the expected level $\sim 30\%$. This, together with the results of a previous paper, provides a coherent picture of bottomonium with $n = 1, 2$ and (to a lesser extent) charmonium with $n = 1$, obtained with calculations from first principles.

PACS number(s): 14.40.Gx, 12.38.Bx, 12.38.Lg, 13.20.Gd

I. INTRODUCTION

In a previous paper [1] (hereafter to be referred as TY[1]) we presented an evaluation of the potential for heavy $q\bar{q}$ systems [1,2]. The evaluation included relativistic effects, one-loop radiative corrections, and (for the spin-independent part) the dominating two-loop ones. With this we evaluated a number of quantities, taking into account also leading nonperturbative corrections, which are known [3] to be due to the contributions of the gluon condensate. It was shown that a very good account could be given of the lowest-lying $b\bar{b}$ bound states (some features of $c\bar{c}$ were also discussed). Notably, both the energy and wave function (this last through e^+e^- decay) of the states with $n = 1$ were given; the splittings between these states and those with $n = 2$, $l = 0, 1$ were reproduced in what is essentially a zero parameter calculation using only the known values of the basic QCD parameters:

$$\begin{aligned}\Lambda(n_f = 4, 2\,\text{loops}) &= 200\ {}^{+80}_{-60}\,\text{MeV}\ ,\\ \langle\alpha_s G^2\rangle &= 0.042 \pm 0.020\ \text{GeV}^4\ ,\\ m_b &= 4906\ {}^{+69}_{-51}\ {}^{-4}_{+4}\ {}^{+11}_{-40}\,\text{MeV}.\end{aligned} \tag{1.1}$$

Actually we preferred in TY to *deduce* m_b from the mass of the $\Upsilon(1S)$ state. The errors given for this quantity in (1.1) correspond to that in Λ (the first), and to that in the gluon condensate (the second); the third is an estimated systematic error.

The value of m_b given in (1.1) is for the *pole* mass, which is the appropriate quantity to be used in a Schrödinger equation. It corresponds to a running mass value of

$$\overline{m}_b(\overline{m}_b^2) = 4397\ {}^{+7}_{-2}\ {}^{-3}_{+4}\ {}^{+16}_{-32}\,\text{MeV}, \tag{1.2}$$

which compares favorably with the Shifman-Vainshtein-Zakharov (SVZ) estimate [4] of $4250 \pm 100\,\text{MeV}$.

For some of the states with $n = 2$, $l = 1, 0$ no result could be given; only the *perturbative* contributions were presented, and they failed to reproduce the experimental values. This was because the nonperturbative corrections, more involved than for the $n = 1$ case, had not been calculated at the time.

In the present paper we finish the calculation of the leading nonperturbative (np) contributions to the $n = 2$ states. We are thus able to present a complete QCD evaluation of the full $n = 1$ and $n = 2$, $l = 1$, 0 bottomonium system. For some of the quantities the np corrections (which are always large) are under control; for some others the calculation loses reliability. In a sense, this paper may be viewed as an attempt to see how far one can go with a perturbative calculation supplemented by leading np effects. We find that, by and large, a coherent picture and good agreement with experiment are obtained. We also profit to correct some of the errors of TY, in particular the neglect of the normalization shift of the wave function due to nonperturbative effects, which, although numerically small, is of conceptual importance.

np corrections grow very fast with n so for $n \geq 3$ they get so large (for $b\bar{b}$) that a QCD calculation based on leading effects becomes meaningless, as was indeed to be expected. However, we present also some results for $n = 3, 4, 5$ with a view to future applications to the $t\bar{t}$ system for which np corrections remain small up to $n \sim 5$.

This paper is organized as follows: the perturbative $q\bar{q}$ Hamiltonian is reproduced in Sec. II for ease of reference. The np corrections to the interaction are evaluated in Sec. III. Sec. IV contains the ensuing shifts in energies and wave functions, which are then applied in Sec. V to the complete evaluation of $n = 1, 2$, $l = 0, 1$, $j = 0, 1, 2$ and spin $s = 0$, 1 bound states of $b\bar{b}$. The article is finished in Sec. VI with numerical results and conclusions.

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[1]We will freely use the notation of TY.

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II. THE PERTURBATIVE QCD POTENTIAL

We present here the Hamiltonian for the $q\bar{q}$ system for ease of reference. We write it separating the spin-independent, LS, tensor, and hyperfine pieces as follows:

$$H_{\rm SI} = H^{(0)} - \frac{C_F\beta_0\alpha_s^2(\mu^2)}{2\pi}\frac{\ln r\mu}{r}, \tag{2.1}$$

$$H^{(0)} = -\frac{1}{m}\Delta - \frac{C_F\widetilde{\alpha}_s(\mu^2)}{r}, \tag{2.2}$$

$$\widetilde{\alpha}_s(\mu^2) = \left[1 + \frac{a_1 + \gamma_E\beta_0/2}{\pi}\alpha_s(\mu^2)\right]\alpha_s(\mu^2), \tag{2.3}$$

$$V_{\rm LS}(\vec{r}) = \frac{3C_F\alpha_s(\mu^2)}{2m^2r^3}\vec{L}\cdot\vec{S} \times\left\{1 + \left[\frac{\beta_0}{2}(\ln r\mu - 1) + 2(1 - \ln mr) + \frac{125 - 10\,n_f}{36}\right]\frac{\alpha_s}{\pi}\right\}, \tag{2.4}$$

$$V_T(\vec{r}) = \frac{C_F\alpha_s(\mu^2)}{4m^2r^3}S_{12}(\vec{r}) \times\left\{1 + \left[D + \frac{\beta_0}{2}\ln r\mu - 3\ln mr\right]\frac{\alpha_s}{\pi}\right\}, \tag{2.5}$$

$$V_{\rm hf}(\vec{r}) = \frac{4\pi C_F\alpha_s(\mu^2)}{3m^2}\vec{S}^2\left\{\delta(\vec{r}) + \left[\frac{\beta_0}{2}\left(\frac{1}{4\pi}{\rm reg}\frac{1}{r^3} + (\ln\mu)\delta(\vec{r})\right) - \frac{21}{4}\left(\frac{1}{4\pi}{\rm reg}\frac{1}{r^3} + (\ln m + B)\delta(\vec{r})\right)\right]\frac{\alpha_s}{\pi}\right\}. \tag{2.6}$$

Here,

$$C_A = 3,\ T_F = 1/2,\ \beta_0 = 11 - \frac{2\,n_f}{3},$$
$$\beta_1 = 102 - \frac{38\,n_f}{3},$$
$$a_1 = \frac{31\,C_A - 20\,T_F\,n_f}{36},$$
$$B = \frac{3}{2}(1 - \ln 2)\,T_F - \frac{5}{9}\,T_F\,n_f + \frac{11\,C_A - 9\,C_F}{18},$$
$$D = \frac{4}{3}\left(3 - \frac{\beta_0}{2}\right) + \frac{65}{12} - \frac{5\,n_f}{18}.$$

${\rm reg}\,r^{-3}$ is defined in TY, $\vec{S} = \vec{S}_1 + \vec{S}_2$ is the total spin, $\vec{L}$ the orbital angular momentum, and

$$S_{12}(\vec{r}) = 2\sum_{ij} S_iS_j\left(\frac{3}{r^2}r_ir_j - \delta_{ij}\right).$$

n_f is the number of *active* flavors. The running coupling constant we take to two loops:

$$\alpha_s(\mu^2) = \frac{4\pi}{\beta_0\ln\mu^2/\Lambda^2}\left\{1 - \frac{\beta_1}{\beta_0^2}\frac{\ln\ln\mu^2/\Lambda^2}{\ln\mu^2/\Lambda^2}\right\}.$$

We have lumped the constant piece of the one-loop correction into $\widetilde{\alpha}_s$ [Eq. (2.3)] because the ensuing potential is still Coulombic and therefore $H^{(0)}$ may still be solved exactly. The relativistic, full one-loop and leading two-loop corrections to the spin-independent piece are known; see TY for details. We will not need them now. The total Hamiltonian is of course

$$H_p = H_{\rm SI} + V_{\rm LS} + V_T + V_{\rm hf}\,, \tag{2.7}$$

where the index p emphasizes that only *perturbative* contributions are taken into account.

A result that we take over from TY is the form of the (spin-independent) wave functions $\bar{\Psi}_{nl}^{(0)}$ pertaining to the Hamiltonian $H_{\rm SI}$. They are easiest obtained with a variational method; one finds that they are given by a formula such as that for the wave functions of the Coulombic Hamiltonian $H^{(0)}$ with the replacement of the "Bohr radius,"

$$a = \frac{2}{mC_F\widetilde{\alpha}_s},$$

by

$$b(n,l) = a\left\{1 + \frac{\ln(n\mu/mC_F\widetilde{\alpha}_s) + \psi(n+l+1) - 1}{2\pi}\beta_0\alpha_s\right\}^{-1}, \tag{2.8}$$

$$\bar{\Psi}_{nl}^{(0)}(\vec{r}) = \Psi_{nl}^{(0)}(\vec{r}; a \to b).$$

A few explicit expressions may be found in Appendix B. In particular the wave function at the origin becomes

$$\Psi_{nl}^{(0)}(0) \to \bar{\Psi}_{nl}^{(0)}(0) = \{1 + \delta_{\rm WF}(n,l)\}\Psi_{nl}^{(0)}(0),$$
$$\delta_{\rm WF}(n,l) = \frac{3\beta_0}{4\pi}\left[\ln\left(\frac{n\mu}{mC_F\widetilde{\alpha}_s}\right) + \psi(n+l+1) - 1\right]\alpha_s. \tag{2.9}$$

As stated, $\Psi_{nl}^{(0)}$ is the solution of the equation

$$H^{(0)}\Psi_{nl}^{(0)} = E_n^{(0)}\Psi_{nl}^{(0)},\qquad E_n^{(0)} = -\frac{(C_F\widetilde{\alpha}_s)^2}{4n^2}m. \tag{2.10}$$

When taking into account the full $H_{\rm SI}$ the energies are shifted to $\bar{E}_{nl}^{(0)}$:

$$\bar{E}_{nl}^{(0)} = E_{nl}^{(0)} - \frac{C_F^2\beta_0\,\alpha_s^2\,\widetilde{\alpha}_s}{4\pi n^2} \times \left\{\ln\frac{n\mu}{mC_F\alpha_s} + \psi(n+l+1)\right\} m\,. \qquad (2.11)$$

A last word about the notation: the superindex (0) in say, $\Psi^{(0)}$, $E^{(0)}$ means "of zero order with respect to *nonperturbative* (np) effects."

III. THE NONPERTURBATIVE INTERACTIONS

It can be shown (TY and [3–5]) that the leading np interactions, *at short distances*, are those associated with the gluon condensate; and, of these, the dominant ones are those where two gluons are attached to the quarks. These interactions are equivalent, in the nonrelativistic limit (including first order relativistic corrections) to those obtained assuming the quarks to move inside a medium of constant, random chromoelectric $\vec{\underset{\sim}{\mathcal{E}}}$ and chromomagnetic $\vec{\underset{\sim}{\mathcal{B}}}$ fields. Because the fields are constant they may be considered to be classical; and because they are random we may take them of zero average value

$$\langle\, \vec{\underset{\sim}{\mathcal{E}}}\,\rangle = \langle\, \vec{\underset{\sim}{\mathcal{B}}}\,\rangle = 0\,.$$

The average is taken in the physical vacuum. Quadratic averages are nonvanishing and may be related to the gluon condensate. With i, j spatial indices and a, b color ones one has (for $N_c = 3$ colors)

$$\langle g^2\mathcal{B}_a^i\mathcal{B}_b^j\rangle = -\langle g^2\mathcal{E}_a^i\mathcal{E}_b^j\rangle = \frac{\pi\delta_{ij}\delta_{ab}}{3(N_c^2-1)}\langle\alpha_s G^2\rangle\,. \qquad (3.1)$$

The relativistic interaction of a quark (labeled with index 1) with classical vector fields may be described by the Dirac Hamiltonian

$$H_{D1} = i\vec{\alpha}_1\cdot\vec{\nabla}_1 - g\gamma\cdot \underset{\sim}{A}(\vec{r}_1) + \beta_1 m\,, \qquad (3.2)$$

$\underset{\sim}{A}^{\mu} = \sum_a \underset{\sim}{t}^{a} A_a^{\mu}$ being gluon fields (in matrix notation). A convenient gauge is that in which

$$\underset{\sim}{A}{}_1^0 = -\vec{r}_1\cdot\vec{\underset{\sim}{\mathcal{E}}},\ \vec{\underset{\sim}{A}}_1 = -\frac{1}{2}\vec{r}_1\times\vec{\underset{\sim}{\mathcal{B}}}.$$

To solve our problem one can apply a Foldy-Wouthuysen transformation [6] to obtain the Hamiltonian (correct including first order relativistic effects)

$$H_{\rm FW1} = m + \frac{1}{2m}(\vec{p}_1 - g\,\vec{\underset{\sim}{A}}_1)^2 - \frac{1}{8m^3}\vec{p}_1^{\,4} - g\vec{r}_1\cdot\vec{\underset{\sim}{\mathcal{E}}} - \frac{g}{m}\vec{S}_1\cdot\vec{\underset{\sim}{\mathcal{B}}} - \frac{g}{2m^2}\vec{S}_1\cdot(\vec{\underset{\sim}{\mathcal{E}}}\times\vec{p}_1)\,, \qquad (3.3)$$

with $\vec{S}_1$ the spin operator and $\vec{p}_1 = -i\vec{\nabla}_1$. Adding to this the Hamiltonian of the antiquark ($g\to -g$, $\vec{r}_1\to\vec{r}_2$) and their interactions given in the previous section we find the full Hamiltonian, which now includes leading np effects. Omitting the trivial rest mass term $2m$, we have

$$H = H^{(0)} - \frac{C_F\beta_0\alpha_s^2}{2\pi}\frac{\ln r\mu}{r} + V_{\rm LS} + V_T + V_{\rm hf} - g\vec{r}\cdot\vec{\underset{\sim}{\mathcal{E}}} + \frac{g}{2m^2}(\vec{S}\times\vec{p})\cdot\vec{\underset{\sim}{\mathcal{E}}} - \frac{g}{m}(\vec{S}_1-\vec{S}_2)\cdot\vec{\underset{\sim}{\mathcal{B}}}. \qquad (3.4)$$

$H^{(0)}$, $V_{\rm LS}$, V_T, $V_{\rm hf}$ are given by Eqs. (2.1) – (2.6). Some of the peculiarities of Eq. (3.4), in particular the absence of an $\vec{L}\cdot\vec{S}$ interaction as well as the presence of a term involving the differences of the spins, had been noted in the similar case of the Zeeman effect in positronium [7]. In Eq. (3.4) we have omitted a term obtained when expanding the square $(\vec{p}_1 - g\,\vec{\underset{\sim}{A}}_1)^2$ in Eq. (3.3), viz., the piece $\vec{\underset{\sim}{A}}{}_1^2$. It would have produced a term $\pi\langle\alpha_s G^2\rangle\, r^2/(48N_c m)$, to be added to Eq. (3.4). The reason for its omission is that it gives *subleading* corrections to all processes (as compared to the contributions of the other terms).

Before embarking upon detailed calculations, let us elaborate on this matter of leading and subleading corrections. Because

$$\langle r\rangle \sim a = \frac{2}{mC_F\widetilde{\alpha}_s}\,,$$
$$\langle p\rangle \sim mv \sim mC_F\widetilde{\alpha}_s\,,$$

it follows that the np terms in Eq. (3.4) are

$$-g\vec{r}\cdot\vec{\underset{\sim}{\mathcal{E}}} \sim \frac{1}{\widetilde{\alpha}_s}\,,\quad \frac{g}{2m^2}(\vec{S}\times\vec{p})\cdot\vec{\underset{\sim}{\mathcal{E}}} \sim \widetilde{\alpha}_s,$$
$$-\frac{g}{m}(\vec{S}_1-\vec{S}_2)\cdot\vec{\underset{\sim}{\mathcal{B}}} \sim (\widetilde{\alpha}_s)^0\,. \qquad (3.5)$$

This simplifies enormously the calculation at the leading order as seldom more than one, and at most two terms, need to be considered. A further simplification is that, with the only exception of the hyperfine splitting for $n = 2$, $l = 1$, only the tree level piece of H_p has to be taken into account when evaluating leading np effects.

IV. ENERGY AND WAVE FUNCTION SHIFTS

A. Spin-independent shifts

Although most of the spin-independent shifts of energies and wave functions were discussed in TY and [3], we give here a detailed calculation for ease of reference, to correct an error common to TY and Leutwyler (cf. Ref. [3]), to present the results for the $n = 2$ wave functions and to explain in this simple case the way the calculation works.

The effects of the nonzero condensate are evaluated with the help of perturbation theory. The perturbation consists of the terms [cf. Eq. (3.4)], $-g\vec{r}\cdot\vec{\underset{\sim}{\mathcal{E}}}$, $\frac{g}{2m^2}(\vec{S}\times\vec{p})\cdot\vec{\underset{\sim}{\mathcal{E}}}$, $-\frac{g}{m}(\vec{S}_1-\vec{S}_2)\cdot\vec{\underset{\sim}{\mathcal{B}}}$. Because, for spin-independent effects, the first term gives a nonzero result we may neglect the others which would contribute corrections of higher order in α_s, cf. Eq. (3.5). Second order perturbation theory is required as only quadratic terms in $\underset{\sim}{\vec{\mathcal{E}}}$ will give a nonvanishing contribution, as discussed in the previous section, Eq. (3.1) and above. The method of evaluation, for this particular case, has been developed by Leutwyler, and independently by Voloshin[2] [3] and is related to Kotani's treatment of the second order Stark effect [8], up to normalization, color, and angular momentum complications that we now discuss.

We denote the solutions of the unperturbed Hamiltonian by

$$H^{(0)}\left|\Psi^{(0)}_{nlM}\right\rangle = E^{(0)}_n\left|\Psi^{(0)}_{nlM}\right\rangle,$$
$$E^{(0)}_n = -\frac{1}{m\,a^2\,n^2} = -\frac{C_F^2\,\widetilde{\alpha}_s}{4\,n^2}\,m,$$
$$\Psi^{(0)}_{nlM} = Y^l_M(\vec{r}/r)\,R^{(0)}_{nl}(r)\,, \tag{4.1}$$

(we have omitted the trivial rest mass energy term). The $R^{(0)}_{nl}(r)$ are identical to the standard Coulombic wave functions for the hydrogen atom with the replacement of the Bohr radius by $a = \dfrac{2}{mC_F\widetilde{\alpha}_s}$. Second order perturbation theory yields immediately the energy and wave function shifts:

$$E = E^{(0)} + E^{\rm np}\,,\quad \Psi = \Psi^{(0)} + \Psi^{\rm np}\,,$$

with

$$E^{\rm np}_{nl} = -\sum_{ij,\,ab}\left\langle \Psi^{(0)}_{nlM}\left| g\,r_i\,\mathcal{E}^i_a\,t^a\,\frac{1}{H^{(0)}-E^{(0)}_n}\,g\,r_j\,\mathcal{E}^j_b\,t^b\right|\Psi^{(0)}_{nlM}\right\rangle \tag{4.2}$$

and

$$\left|\widehat{\Psi}^{\rm np}_{nlM}\right\rangle = \sum_{ij,\,ab} P_{nl}\,\frac{1}{H^{(0)}-E^{(0)}_n}\,P_{nl}\,g\,r_i\,\mathcal{E}^i_a\,t^a\,\frac{1}{H^{(0)}-E^{(0)}_n}\,g\,r_j\,\mathcal{E}^j_b\,t^b\left|\Psi^{(0)}_{nlM}\right\rangle,$$
$$\left|\Psi^{\rm np}_{nlM}\right\rangle = \left|\widehat{\Psi}^{\rm np}_{nlM}\right\rangle + \delta N_{nl}\left|\Psi^{(0)}_{nlM}\right\rangle. \tag{4.3}$$

Here

$$P_{nl} = 1 - \left|\Psi^{(0)}_{nlM}\right\rangle\left\langle\Psi^{(0)}_{nlM}\right|$$

is the projector orthogonal to the nl state. It does not appear in Eq. (4.2) because

$$\langle\Psi^{(0)}_{nlM}|\vec{r}\cdot\underset{\sim}{\vec{\mathcal{E}}}|\Psi^{(0)}_{nlM}\rangle = 0\,.$$

Furthermore, the term $\delta N_{nl}\left|\Psi^{(0)}_{nlM}\right\rangle$ is due to the change in normalization of the wave function induced by the presence of the perturbation. It has been discussed by Voloshin [3]; we will treat it at the end of this section.

The expressions (4.2) and (4.3) are first simplified by replacing

$$g\mathcal{E}^i_a\cdots g\mathcal{E}^j_b \to -\frac{\delta_{ij}\delta_{ab}}{24}\pi\langle\alpha_s G^2\rangle\,, \tag{4.4}$$

recall Eq. (3.1).

Next we take care of the color algebra. The one-gluon exchange potential is given, when acting on arbitrary color states, by

$$-\frac{\alpha_s}{r}\sum_a t^a_{ii'}t^b_{k'k}\,. \tag{4.5}$$

If the initial (and final) states are color singlets we may average

$$\frac{1}{\sqrt{N_c}}\sum_{ik}\delta_{ik}\frac{1}{\sqrt{N_c}}\sum_{i'k'}\delta_{i'k'}\,,$$

and then we get the potential, and Hamiltonian,

$$-\frac{C_F\widetilde{\alpha}_s}{r}\,,\quad H^{(0)} = -\frac{1}{m}\Delta - \frac{C_F\widetilde{\alpha}_s}{r}\,;$$

we have incorporated, as we always do everywhere, the Coulombic piece of the one-loop corrections into $\widetilde{\alpha}_s$.

In Eqs. (4.2) and (4.3), however, the states $\left|\Psi^{(0)}_{nlM}\right\rangle$ are certainly color singlets: hence the matrices t^b (for example) when acting on them will produce a *color octet* state. For a color octet the potential and Hamiltonian are

$$\frac{\widetilde{\alpha}_s}{2N_cr}\,,\quad H'^{(0)} = -\frac{1}{m}\Delta + \frac{\widetilde{\alpha}_s}{2N_cr}\,. \tag{4.6}$$

One then finds

[2] We are grateful to Prof. Y. Simonov for bringing Voloshin's work to our attention.

$$\sum_{ab} \delta_{ab} t^a \frac{1}{H^{(0)} - E_n^{(0)}} t^b \left|\text{singlet}\right\rangle = C_F \frac{1}{H'^{(0)} - E_n^{(0)}} \left|\text{singlet}\right\rangle . \quad (4.7)$$

Putting this together with Eq. (4.4) into Eqs. (4.2) and (4.3) gives the formulas

$$E_{nl}^{\text{np}} = \frac{\pi\langle\alpha_s G^2\rangle}{6N_c} \sum_i \left\langle \Psi_{nlM}^{(0)} \middle| r_i \frac{1}{H'^{(0)} - E_n^{(0)}} r_i \middle| \Psi_{nlM}^{(0)} \right\rangle , \quad (4.8)$$

$$\left|\widehat{\Psi}_{nlM}^{\text{np}}\right\rangle = -\frac{\pi\langle\alpha_s G^2\rangle}{6N_c} P_{nl} \frac{1}{H^{(0)} - E_n^{(0)}} P_{nl} \times \sum_i r_i \frac{1}{H'^{(0)} - E_n^{(0)}} r_i \left|\Psi_{nlM}^{(0)}\right\rangle , \quad (4.9)$$

which takes care of color complications, so we turn to deal with angular momentum. Obviously the perturbation is rotationally invariant so the third component of angular momentum M is not affected by it; but the total angular momentum algebra is not entirely trivial. We write

$$\sum_i r_i \frac{1}{H'^{(0)} - E_n^{(0)}} r_i = \sum_\lambda r_\lambda^* \frac{1}{H'^{(0)} - E_n^{(0)}} r_\lambda ,$$

where $\lambda = 0, \pm 1$, and the r_λ's are spherical components,

$$r_{\pm 1} = \mp \frac{1}{\sqrt{2}}(r_1 \pm i r_2) , \quad r_0 = r_3 .$$

Using the formulas

$$\frac{1}{r} r_\lambda = \sqrt{\frac{4\pi}{3}} Y_\lambda^1(\vec{r}/r)$$
$$\frac{1}{r} r_\lambda^* = (-1)^\lambda \sqrt{\frac{4\pi}{3}} Y_{-\lambda}^1(\vec{r}/r) , \quad (4.10)$$

and the addition theorem for spherical harmonics we get

$$r_\lambda Y_M^l = r \sum_{l'=|l-1|,|l+1|} C_M(l,l',\lambda) Y_{M+\lambda}^{l'} ,$$

$$C_M(l,l',\lambda) = \sqrt{\frac{2l+1}{2l'+1}} (l,M;1,\lambda|l') (l,0;1,0|l') ,$$

with $(\ldots|\ldots)$ the standard Clebsch-Gordan coefficients.

When acting on a function with well-defined angular momentum l we have

$$\frac{1}{H'^{(0)} - E_n^{(0)}} \left|l\right\rangle = \frac{1}{H_l'^{(0)} - E_n^{(0)}} \left|l\right\rangle ,$$
$$\frac{1}{H^{(0)} - E_n^{(0)}} \left|l\right\rangle = \frac{1}{H_l^{(0)} - E_n^{(0)}} \left|l\right\rangle , \quad (4.11)$$

where

$$H_l = -\frac{1}{m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{l(l+1)}{mr^2} + \frac{\kappa\tilde{\alpha}_s}{r} , \quad (4.12)$$

with $\kappa = -C_F$ for $H_l^{(0)}$ and $\kappa = 1/(2N_c)$ for $H_l'^{(0)}$. Using this and the explicit values of the Clebsch–Gordan coefficients we find that Eqs. (4.8) and (4.9) become

$$E_{nl}^{\text{np}} = \frac{\pi\langle\alpha_s G^2\rangle}{6N_c} \frac{1}{2l+1} \left\langle R_{nl}^{(0)} \middle| r \left\{ \frac{l}{H_{l-1}'^{(0)} - E_n^{(0)}} + \frac{l+1}{H_{l+1}'^{(0)} - E_n^{(0)}} \right\} r \middle| R_{nl}^{(0)} \right\rangle , \quad (4.13)$$

$$\left|\widehat{R}_{nl}^{\text{np}}\right\rangle = -\frac{\pi\langle\alpha_s G^2\rangle}{6N_c} \frac{1}{2l+1} P_{nl} \frac{1}{H_l^{(0)} - E_n^{(0)}} P_{nl}\, r \left\{ \frac{l}{H_{l-1}'^{(0)} - E_n^{(0)}} + \frac{l+1}{H_{l+1}'^{(0)} - E_n^{(0)}} \right\} r \left|R_{nl}^{(0)}\right\rangle . \quad (4.14)$$

We have succeeded in separating the color and angular variables to obtain equations involving only the radial variable and radial wave functions. To finish the calculations all that is needed is to find the inverses:

$$\frac{1}{H_l^{(0)} - E_n^{(0)}} \cdots R_{nl}^{(0)} , \quad \frac{1}{H_l'^{(0)} - E_n^{(0)}} \cdots R_{nl}^{(0)} .$$

This is described in Appendix A.

We next turn to the term $\delta N_{nl} \left|\Psi_{nlM}^{(0)}\right\rangle$ in Eq. (4.3). It arises because the presence of the interaction alters the normalization of the $q\bar{q}$ state. This effect was overlooked in the work of Leutwyler [3] and also in TY, but has been discussed in detail by Voloshin [3]. A simple calculation gives that one has to multiply the wave function by

$$\left(1 - \sum_{ij,ab} \left\langle \Psi_{nlM}^{(0)} \middle| g\, r_i\, \mathcal{E}_a^i\, t^a \frac{1}{\left(H^{(0)} - E_n^{(0)}\right)^2} g\, r_j\, \mathcal{E}_b^j\, t^b \middle| \Psi_{nlM}^{(0)} \right\rangle\right)^{1/2}$$
$$\approx 1 + \frac{\pi\langle\alpha_s G^2\rangle}{12N_c} \sum_i \left\langle \Psi_{nlM}^{(0)} \middle| r_i \frac{1}{\left(H'^{(0)} - E_n^{(0)}\right)^2} r_i \middle| \Psi_{nlM}^{(0)} \right\rangle ,$$

and in the second expression we have already carried over the color analysis. After the angular momentum reduction, essentially identical to one performed before, we finally get

$$R_{nl}^{\rm np} = \widehat{R}_{nl}^{\rm np} + \delta N_{nl}\, R_{nl}^{(0)} \,,\tag{4.15}$$
$$\delta N_{nl} = \frac{\pi\langle\alpha_s G^2\rangle}{12N_c}\,\frac{1}{2l+1}\left\langle R_{nl}^{(0)}\right| r\left\{\frac{l}{\left(H_{l-1}^{\prime(0)}-E_n^{(0)}\right)^2} + \frac{l+1}{\left(H_{l+1}^{\prime(0)}-E_n^{(0)}\right)^2}\right\} r\left| R_{nl}^{(0)}\right\rangle .$$

The calculation of the inverses is also described in Appendix A.

The ensuing expressions for the $E_{nl}^{\rm np}$ and $R_{nl}^{\rm np}$ are collected in Appendix B for a few values of n, l and will be employed later on. The expression we get for $E_{nl}^{\rm np}$ agrees with that found by Leutwyler [3] and also $R_{10}^{\rm np}$, the only wave function calculated in Ref. [3], agrees with our evaluation.

We have not succeeded in obtaining a closed general formula for $R_{nl}^{\rm np}$ (for $E_{nl}^{\rm np}$ one is given in Ref. [3]), but a few general properties may be inferred from Eqs. (4.13) and (4.14). Because

$$\langle r\rangle_{nl} \;=\; \frac{a}{2}[3n^2 - l(l+1)] \;\sim\; \frac{n^2}{\widetilde{\alpha}_s}$$

and each energy denominator yields a factor $\frac{n^2}{\widetilde{\alpha}_s^2}$ (see Appendix A) we expect

$$E_{nl}^{\rm np} \sim \frac{n^6}{\widetilde{\alpha}_s^4}\,,\quad R_{nl}^{\rm np} \sim \frac{n^8}{\widetilde{\alpha}_s^6}\,.$$

It thus follows that the importance of nonperturbative effects grows very rapidly with n. Moreover we expect them to be smaller for energies than for wave functions and, generally, to be larger when $l = 0$ than for $l \neq 0$ (for the same value of n). These properties may be verified explicitly in the expressions collected in Appendix B.

The energies and wave functions correct to leading order in np effects and including one-loop corrections are then

$$\begin{aligned} E_{nl} &= \bar{E}_{nl}^{(0)} + E_{nl}^{\rm np}\,,\\ R_{nl}(r) &= \bar{R}_{nl}^{(0)}(r) + R_{nl}^{\rm np}(r)\,,\\ \Psi_{nlM} &= Y_M^l(\vec{r}/r)\,R_{nl}(r)\,,\end{aligned}\tag{4.16}$$

the $\bar{R}^{(0)}$, $\bar{E}^{(0)}$ being as given in Eqs. (2.8) and (2.9).

Finally, we give an expression for the wave function, at all r, for the 10 state, including leading order np and one-loop radiative contributions; this will correct the Eq. (110) of TY, where the normalization shift had been overlooked:

$$\Psi_{10}(\vec{r}) = \frac{1}{(4\pi)^{1/2}}\, f_{10}(r)\,,$$
$$f_{10}(r) = \frac{2}{b^{3/2}}\,e^{-r/b}\left\{1 + \frac{\pi\langle\alpha_s G^2\rangle}{m^4(C_F\widetilde{\alpha}_s)^6}\left(\frac{26712 - 936\rho^2 - 156\rho^3 - 17\rho^4}{3825} + \frac{968\,576}{541\,875}\right)\right\}\,,$$
$$b^{-1} = \frac{mC_F\widetilde{\alpha}_s}{2}\left\{1 + \beta_0\left[\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} - \gamma_E\right]\frac{\alpha_s}{2\pi}\right\}\,,\ \rho = 2\,\frac{r}{b}\,,$$

where $\widetilde{\alpha}_s$ is given in Eq. (2.2).

B. Hyperfine splittings

The hyperfine splittings are caused by the interactions that depend only on spin; they are $V_{\rm hf}$ in Eq. (2.6), and the piece

$$-\frac{g}{m}(\vec{S}_1 - \vec{S}_2)\cdot \underset{\sim}{\vec{B}}$$

in Eq. (3.4). In addition to the splitting caused directly by the last term, there is a nonperturbative contribution indirectly generated by $-g\vec{r}\cdot \underset{\sim}{\vec{\mathcal{E}}}$ .This contribution that we will call "internal," comes about because, when evaluating the expectation values

$$\langle\Psi|\, V_{\rm hf}\,|\Psi\rangle$$

we should use the wave function including the np corrections discussed in the previous subsection:

$$\begin{aligned}\langle\Psi_{nl}|\, V_{\rm hf}\,|\Psi_{nl}\rangle &= \langle\bar{\Psi}_{nl}^{(0)} + \Psi_{nl}^{\rm np}|\, V_{\rm hf}\,|\bar{\Psi}_{nl}^{(0)} + \Psi_{nl}^{\rm np}\rangle\\ &\simeq \langle\bar{\Psi}_{nl}^{(0)}|\, V_{\rm hf}\,|\bar{\Psi}_{nl}^{(0)}\rangle + 2\,\langle\Psi_{nl}^{(0)}|\, V_{\rm hf}\,|\Psi_{nl}^{\rm np}\rangle\,.\end{aligned}\tag{4.17}$$

The internal np splitting is the last term in Eq. (4.17):

$$\Delta_{\rm hf}^{\rm in}\, E_{nls} \;=\; 2\,\langle\Psi_{nl;s}^{(0)}|\, V_{\rm hf}\,|\Psi_{nl;s}^{\rm np}\rangle\,.\tag{4.18}$$

To evaluate this to leading order we use the expression

$$V_{\rm hf} \simeq \frac{4\pi C_F\alpha_s}{3m^2}\,\delta(\vec{r})\vec{S}^{\,2},$$

and thus we get

$$\Delta_{\rm hf}^{\rm in} E_{n0s} = 2s(s+1)\frac{4\pi C_F\alpha_s}{3m^2}\frac{1}{4\pi}R_{n0}^{(0)}(0)\,R_{n0}^{\rm np}(0)\,. \quad (4.19)$$

For $l \neq 0$ the leading piece of $V_{\rm hf}$ gives zero, because $R_{nl}^{(0)}(0)$ vanishes. We have to take into account the radiative correction to $V_{\rm hf}$ and then

$$\Delta_{\rm hf}^{\rm in} E_{nls} = 2s(s+1)\frac{4\pi C_F\alpha_s}{3m^2}\left(\frac{\beta_0}{2}-\frac{21}{4}\right)\frac{1}{4\pi}\frac{\alpha_s}{\pi} \times \int_0^\infty dr\, r^2 R_{nl}^{(0)}(r)\,\frac{1}{r^3}\,R_{nl}^{\rm np}(r)\,,\quad l\neq 0\,. \quad (4.20)$$

It will turn out that, for $l \neq 0$, this internal shift will be subleading. This fact is very interesting because this is one of the few cases where a rigorous QCD analysis yields results *qualitatively* different from the calculations based on phenomenological potentials. This we will discuss in detail elsewhere.

The contribution to hyperfine splitting of the interaction $-\frac{g}{m}(\vec{S}_1-\vec{S}_2)\cdot \underset{\sim}{\vec{\mathcal{B}}}$ we will call "external."[3] It may be calculated as we calculated $E_{nl}^{\rm np}$ in the previous subsection. We find

$$\Delta_{\rm hf}^{\rm ex} E_{nls} = [s(s+1)-3]\,\frac{\pi\langle\alpha_s G^2\rangle}{6N_c m^2}\left\langle R_{nl}^{(0)}\left|\frac{1}{H_l^{'(0)}-E_n^{(0)}}\right|R_{nl}^{(0)}\right\rangle\,. \quad (4.21)$$

The inverse is obtained with the formulas of Appendix A.

To the np contributions we have to add tree level (relativistic) and radiative ones, that we collectively label perturbative: from TY,

$$\Delta_{\rm hf}^{p} E_{n0s} = \frac{s(s+1)}{2}\,\frac{C_F^4\alpha_s(\mu^2)\widetilde{\alpha}_s^3(\mu^2)}{3n^3}\,m[1+\delta_{\rm WF}(n,0)]^2\left\{1+\left[\frac{\beta_0}{2}\left(\ln\frac{n\mu}{mC_F\widetilde{\alpha}_s}-\sum_1^n\frac{1}{k}-\frac{n-1}{2n}\right) - \frac{21}{4}\left(\ln\frac{n}{C_F\widetilde{\alpha}_s}-\sum_1^n\frac{1}{k}-\frac{n-1}{2n}\right)+B\right]\frac{\alpha_s}{\pi}\right\}, \quad (4.22)$$

$$\Delta_{\rm hf}^{p} E_{nls} = \frac{s(s+1)}{2}\,\frac{C_F^4\alpha_s^2\widetilde{\alpha}_s^3}{6\pi n^3 l(l+1)(2l+1)}\left(\frac{\beta_0}{2}-\frac{21}{4}\right)m\,,\quad l\neq 0\,.$$

The constants are as in Eq. (2.6). The full splitting is thus

$$\Delta_{\rm hf} E_{nls} = \Delta_{\rm hf}^{p} E_{nls} + \Delta_{\rm hf}^{\rm in} E_{nls} + \Delta_{\rm hf}^{\rm ex} E_{nls}\,, \quad (4.23)$$

with the various pieces given in Eqs. (4.18)–(4.22).

C. Fine splittings

Also here we have internal and external contributions. The internal ones are, as before, induced by the np modification of the wave function. The calculation is somewhat complicated because now two operators, the LS and Tensor ones [Eqs. (2.4) and (2.5)] contribute. We find[4]

$$\Delta_f^{\rm in} E_{nlj} = 2\delta_{\rm np}(n,l)\left\{\langle V_{\rm LS}^{(0)}\rangle_{nlj}+\langle V_T^{(0)}\rangle_{nlj}\right\}, \quad (4.24)$$

where

$$\delta_{\rm np}(n,l) = \frac{\langle R_{nl}^{(0)}|r^{-3}|R_{nl}^{\rm np}\rangle}{\langle R_{nl}^{(0)}|r^{-3}|R_{nl}^{(0)}\rangle}\,; \quad (4.25)$$

$R_{nl}^{\rm np}$ is given in Eq. (4.14) and $V_{\rm LS}^{(0)}$, $V_T^{(0)}$ are the leading (tree level) pieces of $V_{\rm LS}$, V_T. Using the explicit expressions for these we have

$$\langle V_{\rm LS}^{(0)}\rangle_{nlj} = [j(j+1)-l(l+1)-2] \times \frac{3C_F^4\alpha_s\widetilde{\alpha}_s^3}{16n^3 l(l+1)(2l+1)}\,m\,, \quad (4.26)$$

$$\langle V_T^{(0)}\rangle_{nlj} = \left\langle\frac{1}{2}S_{12}\right\rangle_{jl}\frac{C_F^4\alpha_s\widetilde{\alpha}_s^3}{8n^2 l(l+1)(2l+1)}\,m\,, \quad (4.27)$$

with

$$\left\langle\frac{1}{2}S_{12}\right\rangle_{jl} = \begin{cases} -\frac{l+1}{2l-1}, & j=l-1,\\ +1, & j=l,\\ -\frac{l}{2l+3}, & j=l+1\,.\end{cases} \quad (4.28)$$

The leading external fine structure shift $\Delta_f^{\rm ex} E_{nlj}$ is caused by the crossed combination of the perturbations

$$-g\vec{r}\cdot\underset{\sim}{\vec{\mathcal{E}}},\quad \frac{g}{2m^2}(\vec{S}\times\vec{p})\cdot\underset{\sim}{\vec{\mathcal{E}}}.$$

In this case the external shift is also chromoelectric; the chromomagnetic perturbation $-\frac{g}{m}(\vec{S}_1-\vec{S}_2)\cdot\underset{\sim}{\vec{\mathcal{B}}}$ does not contribute to the fine structure. The color algebra is now like the one for the spin-independent shift, Sec. IV A. Thus,

[3]In the case of hyperfine splittings the internal contribution is chromoelectric and the external one chromomagnetic, but this is not true in other splittings.

[4]We consider that the states correspond to total spin $s=1$. For $s=0$, $\Delta_f^{\rm in} f E_{nlj}^{s=0}=0$.

$$\Delta_f^{\rm ex} E_{nlj} = -2\frac{\pi\langle\alpha_s G^2\rangle}{6N_c}\frac{1}{2m^2}\sum_i \left\langle \Psi_{nlj}^{(0)} \left| (\vec{S}\times\vec{p})_i \frac{1}{H'^{(0)} - E_n^{(0)}} r_i \right| \Psi_{nlj}^{(0)} \right\rangle . \tag{4.29}$$

The angular momentum algebra, on the other hand, is somewhat complicated. It is developed in detail in Appendix C for $n = 2$, $l = 1$. One gets

$$\Delta_f^{\rm ex} E_{21j} = -\frac{\pi\langle\alpha_s G^2\rangle}{6N_c m^2}\left\{ \frac{j(j+1)-4}{2} \left\langle R_{21}^{(0)} \left| \frac{1}{r}\frac{1}{H_2'^{(0)} - E_2^{(0)}} r \right| R_{21}^{(0)} \right\rangle \right.$$
$$\left. + \nu(j) \left\langle R_{21}^{(0)} \left| \frac{\partial}{\partial r}\left(\frac{1}{H_0'^{(0)} - E_2^{(0)}} - \frac{1}{H_2'^{(0)} - E_2^{(0)}} \right) r \right| R_{21}^{(0)} \right\rangle \right\} ,$$
$$\frac{1}{2}\nu(0) = \nu(1) = -\nu(2) = \frac{1}{3} .$$

The calculation is finished using the inverses of Appendix A. The result is

$$\Delta_f^{\rm ex} E_{21j} = \frac{1780\,[j(j+1)-4] - 2784\,\nu(j)}{9945}\,\frac{\pi\langle\alpha_s G^2\rangle}{m^3(C_F\widetilde{\alpha}_s)^2} \equiv K(j)\,\frac{\pi\langle\alpha_s G^2\rangle}{m^3(C_F\widetilde{\alpha}_s)^2} , \tag{4.30}$$

with

$$K(0) = -\frac{8976}{9945} , \quad K(1) = -K(2) = \frac{1}{2}K(0) . \tag{4.31}$$

The perturbative fine splitting is (for $s = 1$; the splitting should be considered to vanish for $s = 0$)

$$\Delta_f^{p} E_{nlj} = \frac{3C_F^4\alpha_s(\mu^2)\widetilde{\alpha}_s^3(\mu^2)}{16n^3 l(l+1)(2l+1)}\, m\,[j(j+1) - l(l+1) - 2]\,[1+\delta_{\rm WF}(n,0)]^2$$
$$\times\left\{ 1 + \left[\left(\frac{\beta_0}{2} - 2\right)\left(\ln n - 1 - \psi(n+l+1) + \psi(2l+3) + \psi(2l) \right.\right.\right.$$
$$\left.\left.\left. - \frac{n-l-1/2}{n}\right) + \frac{125 - 10n_f}{36} + \frac{\beta_0}{2}\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} + 2\ln C_F\widetilde{\alpha}_s \right]\frac{\alpha_s}{\pi} \right\}$$
$$+ \frac{C_F^4\alpha_s(\mu^2)\widetilde{\alpha}_s^3(\mu^2)}{8n^3 l(l+1)(2l+1)}\, m \left\langle \frac{1}{2}S_{12} \right\rangle_{lj} [1+\delta_{\rm WF}(n,0)]^2$$
$$\times\left\{ 1 + \left[D + \left(\frac{\beta_0}{2} - 3\right)\left(\ln n - \psi(n+l+1) + \psi(2l+3) + \psi(2l) \right.\right.\right.$$
$$\left.\left.\left. - \frac{n-l-1/2}{n}\right) + \frac{\beta_0}{2}\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} + 3\ln C_F\widetilde{\alpha}_s \right]\frac{\alpha_s}{\pi} \right\} . \tag{4.32}$$

The constants are as in Eqs. (2.4), (2.5), and (2.9).

The full, relativistic plus radiative plus np fine splitting is then

$$\Delta_f E_{nlj} = \Delta_f^{p} E_{nlj} + \Delta_f^{\rm in} E_{nlj} + \Delta_f^{\rm ex} E_{nlj} , \tag{4.33}$$

the various terms given in Eqs. (4.24), (4.30), and (4.32).

D. Decays into e^+e^-

For a state with $l = 0$ the decay rate into e^+e^- is given by

$$\Gamma(\Upsilon(nS) \to e^+e^-) = \frac{2}{n^3}\left[\frac{Q_b\alpha}{M(\Upsilon(nS))}\right]^2 [mC_F\widetilde{\alpha}_s(\mu^2)]^3$$
$$\times(1+\delta_r)\,[1+\delta_{\rm WF}(n,0)$$
$$+\rho_{\rm np}(n)]^2 . \tag{4.34}$$

Here δ_r is a "hard" radiative correction [9],

$$\delta_r = -\frac{4C_F\alpha_s}{\pi} , \tag{4.35}$$

$\delta_{\rm WF}(n,0)$ is given in Eq. (2.9) and $\rho_{\rm np}(n)$ is the ratio of np to unperturbed wave functions at the origin:

$$\rho_{\rm np}(n) = \frac{R_{n0}^{\rm np}(0)}{R_{n0}^{(0)}(0)} . \tag{4.36}$$

It is to be calculated with the expressions of Appendix B.

V. PROPERTIES OF BOTTOMONIUM IN STATES WITH $n = 1, 2$

We will use spectroscopic notation: states will be labeled $n\,^{2s+1}l_j$, $l = 0, 1, 2 \ldots$ or $S, P, D, \ldots$. The somewhat whimsical notation of the Particle Data Group (PDG) [10] will also be indicated. For $n = 1, 2, 3$ mixing does not occur.

A. States with $n = 1$

From TY we have

$$M(1\,^3S_1) = M(\Upsilon) = 2m\left\{1 - \frac{C_F^2\,\widetilde{\alpha}_s^2(\mu^2)}{8} - \frac{C_F^2\beta_0\,\alpha_s^2(\mu^2)\,\widetilde{\alpha}_s(\mu^2)}{8\pi}\left(\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} + 1 - \gamma_E\right)\right\} + \frac{\epsilon_{10}\pi\langle\alpha_s G^2\rangle}{(mC_F\widetilde{\alpha}_s)^4}\,m\,, \tag{5.1}$$

$$\epsilon_{10} = \frac{1872}{1275} \simeq 1.468\,.$$

The order α_s^4 is partially known;[5] it adds to the right-hand side of Eq. (5.1) a term

$$2m\left[-\frac{3C_F^4}{16}\alpha_s\widetilde{\alpha}_s^3 + \frac{C_F^3 a_2}{8}\,\alpha_s^2\widetilde{\alpha}_s^2 - \frac{5C_F^4}{128}\widetilde{\alpha}_s^4 - \frac{C_F^2\beta_0^2}{16\pi^2}\left(\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} + 1 - \gamma_E\right)^2\alpha_s^3\widetilde{\alpha}_s + \frac{C_F^4}{6}\alpha_s\widetilde{\alpha}_s^3\right]\,. \tag{5.2}$$

We will use both Eq. (5.1) alone and Eqs. (5.1) plus (5.2).

The hyperfine splitting is obtained from Eq. (4.23), $\Delta_{\rm hf}^{\rm in}$ [Eq. (4.19)] evaluated with the expressions for the R's of Appendix B, and the inverse in Eq. (4.21) with those of Appendix A. The result is

$$\begin{aligned}M(1\,^3S_1) - M(1\,^1S_0) &= M(\Upsilon) - M(\eta_b)\\ &= \frac{C_F^4\alpha_s(\mu^2)\widetilde{\alpha}_s^3(\mu^2)}{3}\,m\left\{1 + \left[\frac{\beta_0}{2}\left(\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} - 1\right) - \frac{21}{4}\left(\ln\frac{1}{C_F\widetilde{\alpha}_s} - 1\right) + B\right]\frac{\alpha_s}{\pi}\right\}\\ &\times\left\{1 + \frac{1}{2}\left[\frac{270\,459}{108\,800} + \frac{1\,838\,781}{2\,890\,000} + \frac{1\,161}{8\,704}\right]\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^6} + \frac{3\beta_0}{4}\left(\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} - \gamma_E\right)\frac{\alpha_s}{\pi}\right\}^2 .\end{aligned} \tag{5.3}$$

In the np contribution the first term is the internal, the second the normalization, and the third the external; the last two are, as is generally the case, substantially smaller than the first. The difference in the value of the hyperfine splitting from that in TY, where the normalization shift was overlooked, is fairly small. The corrected value, following from Eq. (5.3), will be given below.

For the e^+e^- decay Eq. (4.34) gives us

$$\begin{aligned}\Gamma(1\,^3S_1 \to e^+e^-) &= \Gamma(\Upsilon \to e^+e^-)\\ &= 2\left[\frac{Q_b\alpha}{M(\Upsilon)}\right]^2\left[mC_F\widetilde{\alpha}_s(\mu^2)\right]^3\left(1 - \frac{4C_F\alpha_s}{\pi}\right)\\ &\times\left[1 + 3\beta_0\left(\ln\frac{\mu}{mC_F\widetilde{\alpha}_s} - \gamma_E\right)\frac{\alpha_s}{4\pi} + \left(\frac{270\,459}{217\,600} + \frac{1\,838\,781}{5\,780\,000}\right)\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^6}\right]^2 ,\end{aligned} \tag{5.4}$$

and we have inserted the explicit values for δ_r, $\delta_{\rm WF}$, $\rho_{\rm np}$.

We also give the decay rate $\Gamma(\eta_b \to 2\gamma)$, which corrects an error in Eq. (95) of TY (a color factor of 3); it is best calculated in terms of the experimental decay $\Gamma^{\rm expt}(\Upsilon \to e^+e^-)$:

$$\Gamma(\eta_b \to 2\gamma) = 3Q_b^2\,\frac{1 - (5 - \pi^2/4)C_F\alpha_s/\pi}{1 - 4C_F\alpha_s/\pi}\,\Gamma^{\rm expt}(\Upsilon \to e^+e^-) \approx 0.51\ {\rm keV}\,.$$

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[5]It includes leading relativistic corrections $O(\alpha_s^4)$, one-loop radiative ones $O((\alpha_s^4/\pi)\ln\mu^2)$ and $O(\alpha_s^4/\pi)$, and leading logarithm two-loop corrections $O((\alpha_s^4/\pi^2)\ln^2\mu^2)$. The error of Eq. (5.2) should be at the 10 to 20 % level.

B. States with $n = 2$, spin-independent shifts, and decay into e^+e^-

We will denote by $\overline{M}(2\,^3P)$ the average of the masses of the states[6] $2\,^3P_j$, $j = 0, 1, 2$:

$$\overline{M}(2\,^3P) = \tfrac{1}{9}\left\{5\,M(2\,^3P_2) + 3\,M(2\,^3P_1) + M(2\,^3P_0)\right\} = 9900 \pm 1 \text{ MeV} . \tag{5.5}$$

From the analysis of TY and Ref. [3] we have

$$\begin{aligned} M(2\,^3S_1) - M(1\,^3S_1) &= M(\Upsilon(2S)) - M(\Upsilon(1S)) \\ &= 2m\left\{\frac{3C_F^2\widetilde{\alpha}_s^2(\mu^2)}{32} + \frac{C_F^2\beta_0\alpha_s\widetilde{\alpha}_s}{32}\left[3\ln\frac{\mu}{C_F m\widetilde{\alpha}_s} + \frac{5}{2} - 3\gamma_E - \ln 2\right]\frac{\alpha_s}{\pi}\right\} \\ &\quad + m\,\frac{(2^6\,\epsilon_{20} - \epsilon_{10})\pi\langle\alpha_s G^2\rangle}{C_F^4 m^4\widetilde{\alpha}_s^4}\,,\quad \epsilon_{20} = \frac{2102}{1326} \simeq 1.585\,, \end{aligned} \tag{5.6}$$

$$\begin{aligned} \overline{M}(2\,^3P) - M(1\,^3S_1) &= 2m\left\{\frac{3C_F^2\widetilde{\alpha}_s^2(\mu^2)}{32} + \frac{C_F^2\beta_0\alpha_s\widetilde{\alpha}_s}{32}\left[3\ln\frac{\mu}{C_F m\widetilde{\alpha}_s} + \frac{13}{6} - 3\gamma_E - \ln 2\right]\frac{\alpha_s}{\pi}\right\} \\ &\quad + m\,\frac{(2^6\,\epsilon_{21} - \epsilon_{10})\pi\langle\alpha_s G^2\rangle}{C_F^4 m^4\widetilde{\alpha}_s^4}\,,\quad \epsilon_{21} = \frac{9929}{9945} \simeq 0.9984\,. \end{aligned} \tag{5.7}$$

It is interesting to consider on its own the "Lamb shift," difference between Eqs. (5.6) and (5.7), as here only the states with $n = 2$ are involved:

$$M(2\,^3S_1) - \overline{M}(2\,^3P) = 2m\,\frac{C_F^2\beta_0\alpha_s^2\widetilde{\alpha}_s}{96\pi} + m\,\frac{2^6\,(\epsilon_{20} - \epsilon_{21})\,\pi\langle\alpha_s G^2\rangle}{C_F^4 m^4\widetilde{\alpha}_s^4}\,. \tag{5.8}$$

As for the decay $\Upsilon(2S) \to e^+e^-$, Eq. (4.34) gives

$$\begin{aligned} \Gamma(2\,^3S_1 \to e^+e^-) &= \frac{1}{4}\left[\frac{Q_b\alpha}{M(\Upsilon(2S))}\right]^2 [mC_F\widetilde{\alpha}_s(\mu^2)]^3\left(1 - \frac{4C_F\alpha_s}{\pi}\right) \\ &\quad \times \left[1 + 3\beta_0\left(\ln\frac{2\mu}{mC_F\widetilde{\alpha}_s} + \frac{1}{2} - \gamma_E\right)\frac{\alpha_s}{4\pi} + \left(\frac{302\,859}{884} + \frac{4\,963\,788}{48\,841}\right)\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^6}\right]^2 . \end{aligned} \tag{5.9}$$

C. States with $n = 2$, fine splittings

From Eq. (4.33) and after some work we get the fine structure splittings[7]

$$\begin{aligned} M(2\,^3P_j) - \overline{M}(2\,^3P) &= m\,C_F^4\,\alpha_s(\mu^2)\,\widetilde{\alpha}_s^3(\mu^2) \\ &\quad \times \left[1 + 3\beta_0\left(\ln\frac{2\mu}{mC_F\widetilde{\alpha}_s} + \frac{5}{6} - \gamma_E\right)\frac{\alpha_s}{4\pi}\right]^2\left(1 + \left(\frac{111\,699}{221} + \frac{145\,137\,762}{1\,221\,025}\right)\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^6}\right) \\ &\quad \times\left\{\frac{j(j+1) - 4}{256}\left\{1 + \left[\left(\frac{\beta_0}{2} - 2\right)\left(\ln\frac{2\mu}{mC_F\widetilde{\alpha}_s} - \gamma_E\right) + 2\ln\frac{\mu}{m} + \frac{125 - 10\,n_f}{36}\right]\frac{\alpha_s}{\pi}\right\}\right. \\ &\quad \left. + \frac{\langle\frac{1}{2}S_{12}\rangle_{1j}}{384}\left\{1 + \left[\left(\frac{\beta_0}{2} - 3\right)\left(\ln\frac{2\mu}{mC_F\widetilde{\alpha}_s} + 1 - \gamma_E\right) + 3\ln\frac{\mu}{m} + D\right]\frac{\alpha_s}{\pi}\right\}\right\} \\ &\quad + m\,\frac{K(j)\,\pi\,\langle\alpha_s G^2\rangle}{m^4(C_F\widetilde{\alpha}_s)^6}\,. \end{aligned} \tag{5.10}$$

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[6]Denoted by $\chi_{bj}(1P)$ by the PDG [10].

[7]Because $\delta_{\rm np}$, $\delta_{\rm WF}$ are large we have included them in a factor $[1 + \delta_{\rm WF}]^2\,(1 + 2\delta_{\rm np})$ in Eq. (5.10). This form or the equivalent one of a factor $[1 + \delta_{\rm WF} + \delta_{\rm np}]^2$ are the ones that give more *stable* numerical results.

The first term containing $\langle\alpha_s G^2\rangle$ is the internal np shift [corresponding to Eq. (4.24)]; the last term is the external piece, Eq. (4.30). The experimental shifts are

$$M(2\,^3P_2) - M(2\,^3P_1) = 21 \pm 1\,\text{MeV}$$
$$M(2\,^3P_1) - M(2\,^3P_0) = 32 \pm 2\,\text{MeV}\,.$$

D. Hyperfine splittings for states with $n = 2$, $l = 1$

The hyperfine splitting $\overline{M}(2\,^3P) - M(2\,^1P_1)$ has not been measured experimentally for bottomonium. For charmonium,

$$\overline{M}_{c\bar{c}}(2\,^3P) - M_{c\bar{c}}(2\,^1P_1) = -0.9 \pm 0.2\,\text{MeV}\,. \quad (5.11)$$

The theoretical calculation has been displayed in Sec. IV B. After substituting the explicit expressions for the various pieces we get

$$\overline{M}(2\,^3P) - M(2\,^1P_1) = m\left(\frac{\beta_0}{2} - \frac{21}{4}\right)\frac{C_F^4\alpha_s^2\widetilde{\alpha}_s^3}{288\pi} + m\,\frac{61}{117}\,\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^2}\,. \quad (5.12)$$

This effect is remarkable. The coefficient $\frac{\beta_0}{2} - \frac{21}{4}$ is *negative*; hence the perturbative and all *internal* np contributions (which are, however, subleading) will be negative. On the other hand, the *external* np correction is *positive.* For the (relatively) light quarks $c\bar{c}$, the perturbative piece dominates; but for $b\bar{b}$, because it decreases like α_s^5, and the np one grows like α_s^{-2}, the situation is reversed and we will get

$$\overline{M}_{b\bar{b}}(2\,^3P) - M_{b\bar{b}}(2\,^1P_1) > 0\,.$$

It should, however, be borne in mind that the prediction Eq. (5.12) is on a much less firm footing than the predictions for $n = 1$. In fact, in our case now, the internal correction Eq. (4.20) although subleading in powers of α_s, is actually (numerically) larger than the nominally leading one, viz., the external contribution in Eq. (4.21). The numerical implications will be discussed in the next section; here we finish with a formula for the 21 hyperfine splitting which takes into account the known pieces of the subleading effects:

$$\overline{M}(2\,^3P) - M(2\,^1P_1) = m\left(\frac{\beta_0}{2} - \frac{21}{4}\right)\frac{C_F^4\alpha_s^2\widetilde{\alpha}_s^3}{288\pi}\left[1 + \frac{3\beta_0}{4\pi}\left(\ln\frac{2\mu}{mC_F\widetilde{\alpha}_s} + \frac{5}{6} - \gamma_E\right)\alpha_s\right]^2 \times [1 + O(\alpha_s)]\left[1 + \left(\frac{111\,699}{221} + \frac{145\,137\,762}{1\,221\,025}\right)\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^2}\right] + m\,\frac{61}{117}\,\frac{\pi\langle\alpha_s G^2\rangle}{m^4\widetilde{\alpha}_s^2}\,[1 + O(\alpha_s)]\,. \quad (5.13)$$

VI. NUMERICAL RESULTS

The numerical results which correspond to the formulas given in the previous sections are presented in Table I. Before discussing them a few words have to be said about the calculational procedure. The quantities pertaining exclusively to $b\bar{b}$ in states with $n = 1$ could have been taken from TY with a small change for the decay $\Upsilon \to e^+e^-$ and the hyperfine Υ-η_b mass difference resulting from the (minute) modification following our corrected evaluation of the np contribution; but we will follow a slightly different path described below. The criterion adopted in TY to choose the renormalization point μ, was to require that radiative and np contributions be equal in absolute value. Most results were in fact little dependent on the actual value of μ chosen. The reason is that, for $n = 1$ the quark mass (as a function of $M(\Upsilon)$ taken as input) begins at order α_s^0 and the first corrections are $O(\alpha_s^2)$. For the decay $\Upsilon \to e^+e^-$, the leading contribution is order α_s^3; finally the "Balmer" mass differences $M(\Upsilon nS) - M(\Upsilon 1S)$ start at order α_s^2. By contrast the Lamb shift $M(2\,^3S_1) - \overline{M}(2\,^3P)$ starts at $O(\alpha_s^3)$, the fine splittings among $2\,^3P_j$ states begin at order α_s^4 (as does the $n = 1$ hyperfine splitting), and, finally, the hyperfine splitting $\overline{M}(2\,^3P) - M(2\,^1P_1)$ is an effect of $O(\alpha_s^5)$. This means that for all these quantities the choice of μ is essential as small variations in μ get amplified. Because of this we have chosen to *fit* the value of μ. We have considered three possibilities: fit the two fine splittings, and then the Lamb shift and Balmer splitting $M(2\,^3S_1) - M(1\,^3S_1)$ come out as predictions; include the Lamb effect in the fit; or fit all four processes. We present results for the last choice because there is little difference among the three, and we consider this last possibility to give the optimum calculation. A remarkable fact that lends credence to our results is that the values of μ obtained with the three methods, as well as with the criterion of TY (for the Lamb shift and Balmer splitting that was considered also there) are extremely close one to another. Moreover, it so happens that the values of μ obtained for $n = 2$ lie very close to what one may call the "natural" scale for $n = 2$ states, viz. the averaged momentum $k_n \equiv \langle\vec{k}^2\rangle_n^{1/2} = mC_F\widetilde{\alpha}_s(k_n)/(2n)$. Indeed, we get $\mu \simeq k_2 \simeq 0.92$ GeV.

For the quantities pertaining to the $n = 1$ states we reproduce the calculations of TY, including the rather small correction due to the inclusion of the normalization shift, overlooked there. The corrected values are given in Table I. It is to be stressed again that, for $n = 1$ states, any choice of μ between 1.2 and 2.5 GeV gives essentially the same results, except for the decay $\Upsilon \to e^+e^-$. Here, and as discussed in TY, we have two scales: k_1 for the

TABLE I. Compilation of results, theoretical predictions, and experimental values for $b\bar{b}$ states with $n = 2$, 1 and $l = 1$, 0, $s = 1$, 0, $j = 0$, 1, 2. The first error is due to the error in Λ, the second to that in $\langle\alpha_s G^2\rangle$.

Quantity	(a)	Experiment
μ (MeV)	$926\ ^{+224}_{-209}\ ^{-47}_{+93}$	
$\alpha_s(\mu^2)$	$0.38\ ^{+0.02}_{-0.02}\ ^{+0.01}_{-0.03}$	
$\widetilde{\alpha}_s(\mu^2)$	$0.55\ ^{+0.05}_{-0.03}\ ^{+0.03}_{-0.05}$	
$2\,^3P_2 - 2\,^3P_1$	$20.6\ ^{+2.6}_{-5.9}\ ^{-2.4}_{+2.2}$	21 ± 1 MeV
$2\,^3P_1 - 2\,^3P_0$	$28.8\ ^{+4.7}_{-8.8}\ ^{-3.1}_{+2.7}$	32 ± 2 MeV
$2\,^3S_1 - \overline{2\,^3P}$	$181\ ^{-38}_{+42}\ ^{+33}_{-43}$	123 ± 1 MeV
$2\,^3S_1 - 1\,^3S_1$	$428\ ^{-98}_{+84}\ ^{+21}_{-32}$	563 ± 0.4 MeV
$\overline{2\,^3P} - 2\,^1P_1$	$1.5\ ^{-0.7}_{+0.4}\ ^{+0.5}_{-0.6}$ MeV	
$\Gamma(2\,^3S_1 \to e^+e^-)$	~ 0.64	0.56 ± 0.10 keV
$\overline{m}_b(\overline{m}_b{}^2)$	$4397\ ^{+7}_{-2}\ ^{-3}_{+4}$ MeV[b]	4250 ± 100[d]
$1\,^3S_1 - 1\,^1S_0$	$36\ ^{+9}_{-7}\ ^{+3}_{-6}$ MeV[c]	
$\Gamma(1\,^3S_1 \to e^+e^-)$	$1.12\ ^{+0.15}_{-0.12}\ ^{+0.14}_{-0.20}$ keV[c]	1.34 ± 0.04
$\Gamma(1\,^3S_1 \to 2\gamma)$	0.51 keV[c]	

[a]Fit (for μ) using $2\,^3P_j$, $2\,^3S_1 - \overline{2\,^3P}$, and $2\,^3S_1 - 1\,^3S_1$. $\left(\chi^2/N_{\rm DF} = \left(0.29\ ^{-0.08}_{+0.62}\ ^{+0.35}_{-0.18}\right)/3\right)$.
[b]Result from TY.
[c]Corrected result with analysis from TY. (For the hyperfine splitting two small errors actually compensate each other).
[d]Values obtained from $e^+e^- \to$ hadrons via QCD sum rules, see Ref. [4].

wave function and m_b^2 for the annihilation. Indeed the criterion of TY gives an intermediate scale $\bar{\mu} = 2.33$ GeV (with the criterion of TY we get: $\delta_r = -0.40$, $\delta_{\rm WF} = -0.19$, and $\delta_{\rm np} = 0.48$). A similar phenomenon occurs for the Balmer splitting where one can fit experiment perfectly using the criterion of TY which yields a scale μ between $k_1 \simeq 1.33$ GeV and k_2.

The values of Λ $\langle\alpha_s G^2\rangle$ were *not* fitted. We chose, as already mentioned,

$$\Lambda(n_f = 3, 2\,\text{loops}) = 250\ ^{+80}_{-70}\ \text{MeV}\,,$$
$$\langle\alpha_s G^2\rangle = 0.042 \pm 0.020\ \text{GeV}^4\,. \quad (6.1)$$

Because we take $M(\Upsilon)$ as input, we *deduce* m_b [and $\bar{m}_b(\bar{m}_b^2)$]. For the pole mass, Eq. (6.1) implies, according to the analysis in TY,

$$m_b = 4906\ ^{+69}_{-51}(\Lambda)\ ^{-4}_{+4}(\langle\alpha_s G^2\rangle)\ \text{MeV}\,, \quad (6.2)$$

the first variation in Eq. (6.2) tied to the variation of Λ in Eq. (6.1), the second tied to that of the gluon condensate also in Eq. (6.1). The results are summarized in Table I.

The agreement between theory and experimental data is remarkable, as is remarkable the stability of the predictions of the (as yet unmeasured) hyperfine splittings. The deviations are of the expected order of the higher corrections, $O(\alpha_s) \sim 30\%$. As drawbacks, however, let us mention the fact that some of the np corrections, notably the ratio $\delta_{\rm np}$, do actually exceed unity.[8] This makes the results of the fine splittings less impressive than what they look at first sight. Nevertheless, the choice of μ as well as the way to write our equations certainly allow a control of the results, for most cases. The hyperfine splitting for $n = 2$, $l = 1$, however, is less stable than the rest. This is because it is the difference between two terms which almost cancel. The central value presented in Table I is 1.7 MeV. If we add subleading corrections as in Eq. (5.13), neglecting the unknown pieces there [the $O(\alpha_s/\pi)$ terms], but we keep $\mu = 926$ MeV, the splitting changes to 0.6 MeV. If, in order to minimize errors caused by subleading terms we adjust μ so that the known subleading pieces of np and perturbative contributions cancel one another we find $\mu = 770$ MeV and a splitting of 1.0 MeV. These variations may be taken as indications of systematic errors in our estimate of this hyperfine splitting.

The process $\Upsilon(2\,^3S_1) \to e^+e^-$ merits a special discussion. If we take the central value $\mu = 926$ MeV [Table I, column(c)] and consider the leading expression of the width, i.e., we neglect radiative and np corrections, we get

[8]A list of some radiative and np contributions is given in Table II.

TABLE II. Sample set of contributions, with μ = 926MeV; $\Lambda(n_f$ = 3, 2 loops) = 250 MeV$\langle\alpha_s G^2\rangle$ = 0.042GeV^4 . All dimensional numbers in MeV.

Quantity	Tree[a]	Tree + rad.[b]	np ext.[c]	$\delta_{\rm WF}$	$\delta_{\rm np}$	Total
$2\,^3P_2 - 2\,^3P_1$	12.5	3.1	1.8	−0.31	2.52	20.6
$2\,^3P_1 - 2\,^3P_0$	15.3	4.6	0.93	−0.31	2.52	28.8

[a]With tree level potential (including relativistic corrections).
[b] Tree level plus one loop radiative corrections.
[c]External np corrections.

$$\Gamma^{(0)} = \frac{1}{4}\left[\frac{Q_b\alpha}{M(2S)}\right]^2 C_F^3 m^3\widetilde{\alpha}_s^3 = 0.64 \text{ keV}. \qquad (6.3)$$

This is the value reported in Table I, and it compares favorably with experiment. Unfortunately the corrections involve the factors

$$(1+\delta_r),\quad [1+\delta_{\rm WF}(2,0)]^2,\quad [1+\rho_{\rm np}(2)]^2$$

[see Eq. (5.9) for the expressions for the δ, ρ], and one has

$$\delta_r = -0.61,\ \delta_{\rm WF} = -0.49,\ \rho_{\rm np} = 5.2.$$

The prediction then becomes meaningless since the corrections are much larger than the nominally leading term, Eq. (6.3); although here, as it happens in the $c\bar{c}$ case (see TY) this leading term yields a reasonable evaluation, considered as an order of magnitude estimate.

Taken all together, our results here as well as those of TY constitute a coherent description of the lowest-lying states of heavy quark systems, using only rigorously derived QCD properties and without need to have recourse to phenomenological potentials or adjustable parameters.

APPENDIX A

We evaluate the inverses

$$\frac{1}{H_l^\kappa - E_n^{(0)}}\rho^\nu e^{-\rho/2} \equiv p_\nu(\rho)e^{-\rho/2}.$$

Here

$$\rho \equiv \frac{2r}{na},\quad E_n^{(0)} = -\frac{1}{ma^2n^2} = -m\frac{C_F^2\widetilde{\alpha}_s^2}{4n^2},$$

$$a = \frac{2}{mC_F\widetilde{\alpha}_s},$$

and

$$H_l^\kappa = -\frac{1}{m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{mr^2} + \frac{\kappa\widetilde{\alpha}_s}{r}.$$

For ν integer p_ν turns out to be a polynomial:

$$p_\nu(\rho) = \sum_{j=0}^{\nu+1} c_j\rho^j,$$

and

$$c_{\nu+1} = \frac{C_F}{\kappa n + (\nu+2)C_F}\frac{mn^2a^2}{4},$$
$$c_{j-1} = \frac{C_F}{\kappa n + jC_F}[j(j+1) - l(l+1)]\,c_j,$$
$$j = l,\ l+1,\ \ldots,\ \nu+1,$$
$$c_j = 0,\quad j<l.$$

When $H_l^\kappa = H_l^{'(0)}$ those equations give a unique well-defined p_ν. For $H_l^\kappa = H_l^{(0)}$ one should replace n by $n+\epsilon$. Then p_ν contains a singular coefficient, proportional to $1/\epsilon$. However, when evaluating

$$\frac{1}{H_l^{(0)} - E_n^{(0)}}P_{nl}\,\rho^\nu e^{-\rho/2}$$

with P_{nl} the projector orthogonal to the solution of

$$\left(H_l^{(0)} - E_n^{(0)}\right)R_{nl}^{(0)} = 0,$$

the singular term drops out and the limit $\epsilon \to 0$ may be taken.

Another useful formula with which reasonably simple, closed expressions for inverses may be obtained is

$$\left(H_l^\kappa + \frac{k^2}{m}\right)R_{Nl}^{(k)}(\rho) = \frac{(2k)^2}{m}\frac{N+l+1+m\kappa\widetilde{\alpha}_s/(2k)}{\rho}\times R_{Nl}^{(k)}(\rho),$$
$$R_{Nl}^{(k)}(\rho) = (\text{const})\rho L_N^{2l+1}(\rho)e^{-\rho/2},$$
$$\rho = 2kr,\ H_l^\kappa \text{ as before}.$$

APPENDIX B

Here we list some nonperturbative energy shifts and wave functions (spin independent). We write

$$E_{nl}^{\rm np} = \frac{\epsilon_{nl}\,n^6\,\pi\langle\alpha_s G^2\rangle}{(mC_F\widetilde{\alpha}_s)^4}m.$$

Then,

$$\epsilon_{10} = \frac{624}{425},\qquad \epsilon_{20} = \frac{1\,051}{663},$$
$$\epsilon_{21} = \frac{9\,929}{9\,945},\qquad \epsilon_{30} = \frac{769\,456}{463\,239},$$
$$\epsilon_{31} = \frac{11\,562\,272}{8\,492\,715},\qquad \epsilon_{40} = \frac{101\,509}{60\,060},$$
$$\epsilon_{50} = \frac{443\,288\,368}{260\,175\,675}.$$

For the wave functions, and with $\rho \equiv \dfrac{2r}{na}$,

$$\widehat{R}_{10}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{2}{a^{3/2}}\,e^{-\rho/2}\left\{\frac{2\,968}{425}-\frac{104}{425}\,\rho^2-\frac{52}{1\,275}\,\rho^3-\frac{1}{225}\,\rho^4\right\},$$

$$\widehat{R}_{20}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{\sqrt{2}\,a^{3/2}}\,e^{-\rho/2}\left\{\frac{3\,828\,736}{1\,989}-\frac{1\,914\,368}{1\,989}\,\rho-\frac{134\,528}{1\,989}\,\rho^2+\frac{67\,264}{5\,967}\,\rho^3+\frac{736}{663}\,\rho^4+\frac{16}{153}\,\rho^5\right\},$$

$$\widehat{R}_{21}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{\sqrt{4!}\,a^{3/2}}\,\rho\,e^{-\rho/2}\left\{\frac{3\,299\,840}{1\,989}-\frac{149\,888}{5\,967}\,\rho^2-\frac{5\,248}{1\,989}\,\rho^3-\frac{32}{153}\,\rho^4\right\},$$

$$\widehat{R}_{30}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{\sqrt{3}\,a^{3/2}}\,e^{-\rho/2}\left\{\frac{189\,965\,808}{5\,719}-\frac{189\,965\,808}{5\,719}\,\rho+\frac{24\,735\,864}{5\,719}\,\rho^2+\frac{3\,462\,552}{5\,719}\,\rho^3\right.$$
$$\left.-\frac{1302}{43}\,\rho^4-\frac{3\,042}{1\,505}\,\rho^5-\frac{9}{43}\,\rho^6\right\},$$

$$\widehat{R}_{31}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{\sqrt{6}\,a^{3/2}}\,e^{-\rho/2}$$
$$\times\left\{\frac{1\,325\,287\,104}{62\,909}\,\rho-\frac{331\,321\,776}{62\,909}\,\rho^2-\frac{124\,833\,216}{314\,545}\,\rho^3+\frac{49\,872}{1\,505}\,\rho^4+\frac{3\,672}{1\,505}\,\rho^5+\frac{9}{43}\,\rho^6\right\},$$

$$\widehat{R}_{40}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{a^{3/2}}\,e^{-\rho/2}\left\{\frac{5\,609\,365\,504}{45\,045}-\frac{2\,804\,682\,752}{15\,015}\,\rho+\frac{57\,706\,496}{1\,001}\,\rho^2-\frac{20\,160\,512}{15\,015}\,\rho^3\right.$$
$$\left.-\frac{93\,551\,104}{135\,135}\,\rho^4+\frac{59\,392}{3\,861}\,\rho^5+\frac{256}{429}\,\rho^6+\frac{32}{351}\,\rho^7\right\},$$

$$\widehat{R}_{50}^{\rm np} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4\,(C_F\widetilde{\alpha}_s)^6}\,\frac{1}{\sqrt{5}\,a^{3/2}}\,e^{-\rho/2}\left\{+\frac{37\,087\,558\,150\,000}{31\,221\,081}-\frac{74\,175\,116\,300\,000}{31\,221\,081}\,\rho+\frac{35\,702\,282\,000\,000}{31\,221\,081}\,\rho^2\right.$$
$$\left.-\frac{13\,695\,312\,550\,000}{93\,663\,243}\,\rho^3-\frac{561\,983\,427\,500}{93\,663\,243}\,\rho^4+\frac{138\,527\,387\,500}{93\,663\,243}\,\rho^5-\frac{4\,827500}{261\,873}\,\rho^6-\frac{1\,250}{9\,699}\,\rho^7-\frac{625}{6\,588}\,\rho^8\right\}.$$

For ease of reference we also give the first $R^{(0)}$'s

$$R_{10}^{(0)}(r) = \frac{2}{a^{3/2}}\,e^{-r/a},$$
$$R_{20}^{(0)}(r) = \frac{1}{\sqrt{2}\,a^{3/2}}\left(1-\frac{r}{2a}\right)e^{-r/2a},$$
$$R_{21}^{(0)}(r) = \frac{1}{\sqrt{4!}\,a^{3/2}}\,\frac{r}{a}\,e^{-r/2a}.$$

For the $\bar{R}_{nl}^{(0)}$'s, replace a by $b(n,l)$ given in Eq. (2.8). Moreover,

$$R_{nl}^{\rm np} = \widehat{R}_{nl}^{\rm np} + (\delta N_{nl})\,R_{nl}^{(0)}\,,$$
$$\delta N_{nl} = \frac{\pi\langle\alpha_s G^2\rangle}{m^4(C_F\widetilde{\alpha}_s)^6}\,c_{nl}\,,$$

with

$$c_{10} = \frac{968\,576}{541\,875}, \qquad c_{20} = \frac{753\,025\,024}{1\,318\,707},$$
$$c_{21} = \frac{33\,026\,904\,064}{98\,903\,025}, \qquad c_{30} = \frac{156\,976\,204\,684}{9\,556\,977},$$
$$c_{31} = \frac{163\,321\,569\,554}{12\,756\,175}, \qquad c_{40} = \frac{1\,212\,380\,677\,586}{7\,072\,153},$$
$$c_{50} = \frac{2\,837\,889\,485\,981}{2\,721\,892}\,.$$

A closed expression may be obtained for the c_{n0} with the help of the last formula of the previous Appendix.

APPENDIX C

We evaluate the matrix element (21 stands for nl)

$$\mathcal{M} = \sum_i \left\langle \Psi_{21j}^{(0)} \left| \left(\vec{S}\times\vec{P}\right)_i \frac{1}{H'^{(0)}-E_2^{(0)}}\, r_i \right| \Psi_{21j}^{(0)} \right\rangle .$$

It is convenient to use a Cartesian basis for the spin-angular momentum piece of $\Psi_{21j}^{(0)}$ so that

$$\Psi_{21j}(\vec{r}) = \sum_{ik} \xi_{ik}^{(\alpha)}(j)\,\hat{r}_i\,\underset{\sim}{\chi}_k R_{21}^{(0)}(r)\,. \qquad \text{(C1)}$$

Here $\hat{r} = \vec{r}/r$, the $\underset{\sim}{\chi}_k$ are column spin 1 wave functions and the coefficients $\xi_{ik}^{(\alpha)}(j)$ are

$$\xi_{ik}^{(0)}(0) = \frac{1}{\sqrt{4\pi}}\,\delta_{ik}\,, \quad \xi_{ik}^{(a)}(1) = \frac{3}{\sqrt{8\pi}}\,\epsilon_{aik}\,,$$
$$\xi_{ik}^{(ab)}(2) = \frac{3}{\sqrt{4\pi}}\left\{\delta_{ia}\,\delta_{kb}-\frac{1}{3}\,\delta_{ik}\,\delta_{ab}\right\}.$$

The last expression valid for $a \neq b$. The indices 0, a, ab, collectively denoted by α in (3.1) give the (Cartesian) third component of total angular momentum. The spin-angular momentum wave functions

$$\underset{\sim}{\xi}^{(\alpha)}(j) = \sum_{ik} \xi_{ik}^{(\alpha)}(j)\ \hat{r}_i\ \underset{\sim}{\chi}_k$$

form an orthonormal set:

$$\int d\Omega\ \underset{\sim}{\xi}^{(\alpha)}(j)\ \underset{\sim}{\xi}^{(\beta)}(j') = \delta_{jj'}\,\delta_{\alpha\beta}\ .$$

We have

$$\mathcal{M} = \sum_a \left\langle R_{21}^{(0)}\ \underset{\sim}{\xi}(j) \middle| \left(\vec{S}\times\vec{P}\right)_a \frac{1}{H'^{(0)} - E_2^{(0)}}\ r_a \middle| R_{21}^{(0)}\ \underset{\sim}{\xi}(j)\right\rangle$$
$$= \sum_{\substack{ik\,i'k'\\abc}} \left\langle R_{21}^{(0)} \middle| \int d\Omega\ \xi_{i'k'}(j)\,\hat{r}_{i'}\ \underset{\sim}{\chi}_{k'}^{\dagger}\epsilon_{abc}S_b\,P_c \frac{1}{H'^{(0)} - E_2^{(0)}} r_a\,\hat{r}_i\xi_{ik}(j)\ \underset{\sim}{\chi}_k \middle| R_{21}^{(0)}\right\rangle .$$

If we write identically

$$\hat{r}_a\hat{r}_i\ =\ \left(\hat{r}_a\hat{r}_i - \frac{1}{3}\,\delta_{ai}\right) + \frac{1}{3}\,\delta_{ai}\ ,$$

then the first term corresponds to angular momentum 2, and the second to angular momentum zero. Therefore, when acting on the first we may replace $H'^{(0)}$ by $H_2'^{(0)}$, and when acting on the second $H'^{(0)}$ by $H_0'^{(0)}$. Hence,

$$\mathcal{M} = \sum_{\substack{ik\,i'k'\\abc}} \left\langle R_{21}^{(0)} \middle| \int d\Omega\ \xi_{i'k'}\,\hat{r}_{i'}\ \underset{\sim}{\chi}_{k'}^{\dagger}\epsilon_{abc}\,S_b\,P_c \left(\hat{r}_a\hat{r}_i - \frac{1}{3}\,\delta_{ai}\right) \frac{1}{H_2'^{(0)} - E_2^{(0)}}\xi_{ik}\ \underset{\sim}{\chi}_k r \middle| R_{21}^{(0)}\right\rangle$$
$$+ \frac{1}{3} \sum_{\substack{ik\,i'k'\\abc}} \left\langle R_{21}^{(0)} \middle| \int d\Omega\ \xi_{i'k'}\,\hat{r}_{i'}\ \underset{\sim}{\chi}_{k'}^{\dagger}\epsilon_{abc}\,S_b\,P_c\,\delta_{ai} \frac{1}{H_0'^{(0)} - E_2^{(0)}}\ \xi_{ik}\ \underset{\sim}{\chi}_k r \middle| R_{21}^{(0)}\right\rangle\ ,$$

and, after straightforward substitutions and arrangements,

$$\mathcal{M} = \sum_{ik\,i'k'} \left\langle R_{21}^{(0)} \middle| \int d\Omega\ \xi_{i'k'}\,\hat{r}_{i'}\ \underset{\sim}{\chi}_{k'}^{\dagger}\vec{S}\cdot\vec{L}\ r_i\,\frac{1}{r}\ \frac{1}{H_2'^{(0)} - E_2^{(0)}}\ \xi_{ik}\ \underset{\sim}{\chi}_k r \middle| R_{21}^{(0)}\right\rangle$$
$$+ \frac{1}{3} \sum_{ik\,i'k'\,cs} (\delta_{is}\,\delta_{ck} - \delta_{ik}\,\delta_{cs}) \left\langle R_{21}^{(0)} \middle| \int d\Omega\ \xi_{i'k'}\,\hat{r}_{i'}\ \underset{\sim}{\chi}_{k'}^{\dagger}\xi_{ik}\,\hat{r}_c\,\chi_s\,\frac{\partial}{\partial r}\left(\frac{1}{H_0'^{(0)} - E_2^{(0)}} - \frac{1}{H_2'^{(0)} - E_2^{(0)}}\right) r \middle| R_{21}^{(0)}\right\rangle .$$

The only noteworthy aspects of the derivation are first, that, because $H_l'^{(0)}$ only acts on the radial variable, and the $\hat{r}_i$ only depend on the angular ones,

$$\frac{1}{H_l'^{(0)} - E_2^{(0)}}\,\hat{r}_i\ =\ \hat{r}_i\,\frac{1}{H_l'^{(0)} - E_2^{(0)}}\ ,$$

and, second, that for any $f(r)$,

$$P_k\,f(r)\ =\ -i\,\hat{r}_k\,\frac{\partial f(r)}{\partial r}\ .$$

The calculation is readily finished. Because

$$\sum_{ik} \xi_{ik}(j)\ \hat{r}_i\ \underset{\sim}{\chi}_k$$

corresponds to total angular momentum j,

$$\vec{S}\cdot\vec{L}\ \sum_{ik} \xi_{ik}(j)\ \hat{r}_i\ \underset{\sim}{\chi}_k = \frac{j(j+1) - l(l+1) - s(s+1)}{2}\ \sum_{ik} \xi_{ik}(j)\ \hat{r}_i\ \underset{\sim}{\chi}_k,$$

with $l = s = 1$. Defining also

$$\nu(j) = \frac{4\pi}{9} \sum_{ik} [\xi_{ik}(j)\xi_{ki}(j) - \xi_{ii}(j)\xi_{kk}(j)] ,$$
$$\frac{1}{2}\nu(0) = \nu(1) = -\nu(2) = \frac{1}{3} ,$$

we finally get

$$\mathcal{M} = \frac{4 - j(j+1)}{2} \left\langle R_{21}^{(0)} \middle| \frac{1}{r} \frac{1}{H_2^{'(0)} - E_2^{(0)}} r \middle| R_{21}^{(0)} \right\rangle + \nu(j) \left\langle R_{21}^{(0)} \middle| \frac{\partial}{\partial r} \left(\frac{1}{H_0^{'(0)} - E_2^{(0)}} - \frac{1}{H_2^{'(0)} - E_2^{(0)}} \right) r \middle| R_{21}^{(0)} \right\rangle .$$

Note added: A few typographical errors crept in TY that we now correct; Eqs. (34), (39), (62), (67), and (68) should read

$$\delta \widetilde{V}_4^{(2)} = \frac{-4\pi C_F \alpha_s(\mu^2)}{k^2} \left[\frac{\beta_0^2}{4} \ln^2 \frac{k}{\mu} - \frac{\beta_1}{8} \ln \frac{k}{\mu} + \text{const} \right] \frac{\alpha_s^2(\mu^2)}{\pi^2} , \tag{34}$$

$$\delta V_4^{(2)}(r) = -\frac{C_F \beta_0^2 \alpha_s^3}{4\pi^2} \frac{\ln^2 \mu r}{r} - \left[\frac{\gamma_E \beta_0^2}{2\pi^2} + \frac{\beta_1}{8\pi^2} \right] C_F \alpha_s^3 \frac{\ln \mu r}{r} - \left[\frac{\gamma_E{}^2 \beta_0^2}{4\pi^2} + \frac{\beta_0^2}{48} + \frac{\beta_1 \gamma_E}{8\pi^2 \beta_0} + \text{const} \right] C_F \alpha_s^3 \frac{1}{r} , \tag{39}$$

$$A_3(n,l) = -\frac{C_F \beta_0 \alpha_s^2}{4n^2 \pi m a} \left\{ \ln \frac{n a \mu}{2} + \psi(n+l+1) \right\} , = -\frac{C_F^2 \beta_0 \alpha_s^2 \widetilde{\alpha}_s}{8\pi n^2} \left\{ \ln \frac{n\mu}{m C_F \widetilde{\alpha}_s} + \psi(n+l+1) \right\} , \tag{62}$$

$$A_5(n=1, l=0) = -\frac{3C_F^4 \beta_0}{32\pi} \left[\ln \frac{\mu}{m C_F \widetilde{\alpha}_s} - \frac{1}{3} - \gamma_E \right] \alpha_s^2 \widetilde{\alpha}_s^3 - \frac{C_F^4 a_3}{16\pi} \left[\ln \frac{1}{m C_F \widetilde{\alpha}_s} - 1 \right] \alpha_s^2 \widetilde{\alpha}_s^3 + \frac{C_F^4 \left[a_5 - (5/6 + \ln \bar{n})\, a_4 \right]}{16\pi} \alpha_s^2 \widetilde{\alpha}_s^3 , \tag{67}$$

$$A_S(n,0,s) = \delta_{s1} \frac{C_F^4 \alpha_s \widetilde{\alpha}_s^3}{6n^3} \left\{ 1 + \left[\frac{\beta_0}{2} \left(\ln \frac{n\mu}{m C_F \widetilde{\alpha}_s} - \sum_1^n \frac{1}{k} - \frac{n-1}{2n} \right) - \frac{21}{4} \left(\ln \frac{n}{C_F \widetilde{\alpha}_s} - \sum_1^n \frac{1}{k} - \frac{n-1}{2n} \right) + B \right] \frac{\alpha_s}{\pi} \right\} + A_{\mathrm{S,np}} . \tag{68}$$

This work is partially supported by CICYT, Spain.

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