Color-hyperfine splitting in heavy-quarkonium P states from perturbative QCD with a running coupling strength

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We obtain an expression for the color-hyperfine interaction in heavy quarkonium in perturbative QCD including terms up to one loop, but going beyond one loop by letting the strong-interaction coupling constant α_s run. The resulting expression cannot be written analytically in position space, but we make approximations which enable us to obtain approximate upper and lower bounds on the P-wave color-hyperfine splittings in charmonium and bottomonium.

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Recently, there has been renewed theoretical interest in the masses of the ^1P states in charmonium and bottomonium [1–3]. Calculations [1–9] find that a given ^1P state in heavy quarkonium lies very close to the center of gravity of the corresponding ^3P states. However, different theoretical methods yield opposite values for the sign of the splitting. In this paper we modify a one-loop perturbative QCD calculation of Gupta *et al.* [4] and Pantaleone *et al.* [5] by letting the coupling constant α_s run. Because certain terms in the expression for the color-hyperfine splitting vanish in P states if α_s is fixed, we find that our results are sensitive to whether we let α_s run. We let M_3 be the mass of the center of gravity of the ^3P states, M_1 be the mass of the ^1P state, and $\Delta M_P = M_3 - M_1$. We call ΔM_{Ph} the contribution to ΔM_P arising from the color-hyperfine interaction. This is the only contribution we calculate in this paper.

There is a simple reason why the procedures of keeping α_s fixed and letting it run can lead to quite different results for the P-wave hyperfine splitting. Whereas in S states the lowest-order (one-gluon-exchange) contribution is dominant and leads to the ^3S state lying higher than the ^1S state, in states with orbital angular momentum L different from zero the one-gluon-exchange contribution (with fixed α_s) vanishes. Therefore, in P states with α_s fixed, the one-loop contribution is dominant and its sign is such [4,5] as to make the mass M_1 be *larger* than M_3, i.e., $\Delta M_{Ph} < 0$. However, if α_s runs, the one-gluon-exchange contribution does not vanish in P states, and so the sign of ΔM_{Ph} is not obvious.

In this paper, we reexamine what one-loop perturbative QCD says about the P-wave color-hyperfine splitting, concentrating on the effect of the running coupling constant. We find that if α_s is allowed to run, the one-gluon-exchange contribution acts to lower the singlet P state with respect to the center of gravity of the corresponding triplet states; i.e., at the tree level with running coupling constant, we obtain $\Delta M_{Ph} > 0$. The splitting is very small, however, and so might be reversed at the one-loop level.

Because our one-loop expression with running α_s is complicated, we consider two approximations to ΔM_{Ph}, one of which overestimates this quantity and the other of which underestimates it. By so doing, we find approximate upper and lower limits on ΔM_{Ph}, which, in the case of charmonium, differ by about 8 MeV, and, in the case of bottomonium, differ by about 2 MeV. Our upper and lower limits also differ in sign.

According to QCD perturbation theory, the spin-dependent interactions in heavy quarkonium consist of a spin-spin or color-hyperfine interaction, a tensor interaction, and a spin-orbit interaction. If we treat the spin-dependent interactions in heavy quarkonium as small perturbations, then the effects of the tensor and spin-orbit interactions cancel when taking the center of gravity ^3P of the $^3P_2$, $^3P_1$, and $^3P_0$ states ($\frac{5}{9}\,^3P_2 + \frac{3}{9}\,^3P_1 + \frac{1}{9}\,^3P_0$). In this approximation, and if coupled-channel and other small effects are neglected, the splitting of the ^3P from the ^1P levels is a measure of the color-hyperfine splitting ΔM_{Ph}.

In QCD perturbation theory the color-hyperfine interaction H_h can be written

$$H_h = Y(r)\mathbf{S}_1\cdot\mathbf{S}_2 \,, \tag{1}$$

where $\mathbf{S}_1$ and $\mathbf{S}_2$ are the spins of the quark and antiquark and $Y(r)$ depends on the quark masses as well as the quark-antiquark separation r. Then ΔM_{Ph} is given by

$$\Delta M_{Ph} = \langle P|Y(r)|P\rangle \,, \tag{2}$$

where $\langle P|Y|P\rangle$ denotes the expectation value of Y with respect to the unperturbed P-wave function.

In the Fermi-Breit (FB) approximation [10], $Y(r)$ is given by

$$Y_{\rm FB}(r) = (32\pi/9)\alpha_s\delta(\mathbf{r})/m^2 \,, \tag{3}$$

where α_s is the strong-interaction coupling strength and we are restricting ourselves to a quark and antiquark which both have the same mass m. Equation (3) follows from the fact that the one-gluon-exchange diagram with a fixed α_s gives rise to a static Coulomb potential. (By the static potential we mean the potential in the limit of

infinitely heavy quarks.) We see from Eqs. (2) and (3) that $\langle Y_{\rm FB}(r)\rangle$ vanishes in P states, owing to the fact that the wave function of a P state vanishes at the origin. Therefore, according to the FB approximation, ΔM_{Ph} is zero.

If, for any reason, the static quark-antiquark potential is not of Coulomb form, the FB expression can be generalized [11,12] to the form

$$Y_{\rm GBF}(r)=(2/3m^2)\nabla^2 V(r)\ , \tag{4}$$

where $V(r)$ is that part of the quark-antiquark static potential which transforms as the time component of a four-vector. Although expression (4) is usually just called the Fermi-Breit approximation, we call it the generalized Fermi-Breit (GFB) approximation. In this paper we assume that $V(r)$ can be calculated in perturbative QCD, i.e., that the confining potential transforms like a Lorentz scalar.

In the one-gluon-exchange approximation, $V(r)$ is given by

$$V(r)=-4\alpha_s/(3r)\ . \tag{5}$$

If in Eq. (5) α_s is a constant, then Eq. (4) reduces to Eq. (3). However, if α_s is allowed to run as a function of r, then the potential is not of Coulomb form, and Eq. (4) applies.

Now we know from experiment that the S-wave splitting ΔM_S is greater than zero, and therefore it follows in the GFB approximation that

$$\langle S|\nabla^2 V|S\rangle>0\ . \tag{6}$$

The inequality (6) is a consequence of the stronger condition

$$\nabla^2 V(r)>0 \quad \text{for all } r\ , \tag{7}$$

but of course, it is not necessary that (7) be true in order for (6) to hold. However, if (7) holds, then it follows in the GFB approximation that $\Delta M_{Ph}>0$. Later, we shall explicitly show that the inequality (7) is true for a class of asymptotically free running couplings.

Eichten and Feinberg [13], Gromes [14], and Dine [15] have gone beyond the GFB approximation in QCD. Whereas, in the GFB approximation $Y(r)$ is directly given in terms of derivatives of $V(r)$ by Eq. (4), in the formulation of Eichten, Feinberg, Dine, and Gromes, additional functions of r, not given in terms of $V(r)$, enter into the expression for $Y(r)$. Gupta and Radford [16], Gupta *et al.* [4], and Pantaleone *et al.* [5] have computed these additional terms in QCD perturbation theory at the one-loop level with fixed α_s.

Let us call $y(Q)$ the Fourier transform of $Y(r)$. The expression of Gupta *et al.* [4] and Pantaleone *et al.* [5] for $y(Q)$ is

$$y(Q)=\frac{32\pi\alpha_s}{9m^2}\mathcal{F}-\frac{4\alpha_s^2}{3m^2}\left[\frac{16}{9}+2\ln 2-7\ln\frac{Q^2}{m^2}\right], \tag{8}$$

where Q is the magnitude of the three-momentum and α_s is evaluated at a scale μ. Here $\mathcal{F}$ is given by

$$\mathcal{F}=1-\frac{\alpha_s}{12\pi}\left[(33-2n_f)\ln\frac{Q^2}{\mu^2}+\xi\right], \tag{9}$$

where n_f is the effective number of quark flavors and ξ is a constant which depends on the renormalization scheme. In the modified minimal-subtraction ($\overline{\rm MS}$) scheme [17] used by Pantaleone *et al.*, $\xi=10n_f/3-31$ ($\xi=-21$ for three flavors), whereas in the renormalization scheme used by Gupta *et al.*, $\xi=+18$.

It can be deduced from Eq. (8) that for fixed $\alpha_s(\mu)$ the lowest-order term (the term linear in α_s) vanishes in P states (this is the FB approximation). Furthermore, the sum of the α_s^2 terms, which arise from QCD in one-loop diagrams, is *negative* in the calculations of Gupta *et al.* [4] and Pantaleone *et al.* [5]. Therefore, these authors find that ΔM_{Ph} is negative. The magnitude of the splitting turns out to be a few MeV in charmonium and 1 MeV or less in bottomonium [4–6]. Igi and Ono [9], who also calculate to order one loop, obtain the same result (see the erratum to their paper).

The starting point of our calculation is Eq. (8). However, rather than let α_s be fixed at some value $\alpha_s(\mu)$, we let (at least) one power of α_s run as a function of Q. Dine [15] also let one power of α_s run, but his expression omitted some terms contained in Eq. (8). Also, he did not put his result in a form which enabled him to compare with experiment.

Once we let α_s run, we have to change the factor $\mathcal{F}$ of Eq. (9) to avoid double counting. The term $\alpha_s(33-2n_f)\ln(Q^2/\mu^2)/12\pi$ in $\mathcal{F}$ is the second-order term in the expansion of $\alpha_s(Q)$, so we omit it. Also, it turns out that our qualitative results are not sensitive to the renormalization-scheme-dependent quantity ξ. We remark here that we use the $\overline{\rm MS}$ scheme, in which ξ is negative, so that it gives a small *positive* contribution to ΔM_{Ph}. Thus, in Eq. (8) we simply use

$$\mathcal{F}=1-\alpha_s(Q)\xi/12\pi\ . \tag{10}$$

Then Eq. (8) becomes

$$y(Q)=\frac{32\pi\alpha_s(Q)}{9m^2}\left[1+\frac{3\alpha_s(Q)}{8\pi}\left[7\ln\frac{Q^2}{m^2}-\frac{16}{9}-2\ln 2-\frac{2}{9}\xi\right]\right]. \tag{11}$$

It is straightforward to find $Y(r)$ numerically by taking the Fourier transform of $y(r)$ as given in Eq. (11), provided we choose an expression for $\alpha_s(Q)$ which does not diverge at small Q. One possibility is to use the following approximation for the running coupling constant:

$$\alpha_s(Q)=\frac{12\pi}{(33-2n_f)\beta}\left[1-\frac{6(153-19n_f)\ln\beta}{(33-2n_f)^2\beta}\right], \tag{12}$$

where

$$\beta=\ln[(Q^2/\Lambda^2)+\kappa] \tag{13}$$

and κ is a parameter satisfying $\kappa>1$. We introduce the parameter κ so that α_s is finite for all Q^2. If $Q^2\gg\kappa\Lambda^2$,

then our expression for α_s reduces to the usual second-order result [17].

In the one-gluon approximation with running coupling, the potential $V(r)$ is given by

$$V(r)=-\frac{2}{3\pi^2}\int\frac{\alpha_s(Q)}{Q^2}\exp(i\mathbf{Q}\cdot\mathbf{r})d\mathbf{Q}\ . \tag{14}$$

We can define $\alpha_s(r)$ by the equation

$$-\frac{4\alpha_s(r)}{3r}=V(r)\ , \tag{15}$$

where $V(r)$ is given by (14). Using the $\alpha_s(Q)$ of Eq. (12) with a variety of reasonable values of κ in the range $1.3\le\kappa\le 3.0$, we have obtained the Fourier transform (14) numerically. We find that $\alpha_s(r)$ satisfies the following properties for all r relevant to our problem, i.e., for all r for which the charmonium and bottomonium wave functions have appreciable support:

$$\alpha_s(r)>0,\quad \alpha_s'(r)>0,\quad \alpha_s''(r)<0\ , \tag{16}$$

where the prime denotes the derivative with respect to r. We can easily see that (7) holds wherever the third of the conditions in (16) holds, which is to say, for all relevant values of r.

We now consider two approximation methods which enable us to write the splitting in terms of modified GFB formulas. By so doing, we obtain expressions which enable us to obtain approximate bounds on ΔM_{Ph}.

It is convenient to use the identity

$$\ln\frac{Q^2}{m^2}=\ln\frac{Q^2}{\Lambda^2}-\ln\frac{m^2}{\Lambda^2}\ , \tag{17}$$

where Λ is the QCD scale parameter. Equation (11), with the identity (17), is the starting point for both of our approximation methods.

(1) In our first method, we begin by approximating $\ln(Q^2/\Lambda^2)$ and $\ln(Q^2/m^2)$ by the lowest-order expressions

$$\ln\frac{Q^2}{\Lambda^2}=\frac{12\pi}{33-2n_f}\frac{1}{\alpha_s(Q)}\ ,\qquad \ln\frac{m^2}{\Lambda^2}=\frac{12\pi}{33-2n_f}\frac{1}{\alpha_s(m)}\ . \tag{18}$$

Then Eq. (11) becomes

$$y(Q)=\frac{32\pi\alpha_s(Q)}{9m^2}\left[1+\frac{63}{2(33-2n_f)}\left[1-\frac{\alpha_s(Q)}{\alpha_s(m)}\right]-\frac{3\alpha_s(Q)}{4\pi}\left[\frac{8}{9}+\ln 2+\frac{\xi}{9}\right]\right]\ . \tag{19}$$

For a reasonable choice of $\alpha_s(Q)$ we are unable to take the Fourier transform of $y(Q)$ analytically. However, let us make the approximation of replacing $\alpha_s(Q)$ appearing within the square brackets in Eq. (19) by $\alpha_s(\mu)$, and define x to be

$$x=\frac{63}{2(33-2n_f)}\left[\frac{\alpha_s(\mu)}{\alpha_s(m)}-1\right]+\frac{3\alpha_s(\mu)}{4\pi}\left[\frac{8}{9}+\ln 2+\frac{\xi}{9}\right]\ . \tag{20}$$

Then $y(Q)$ becomes

$$y(Q)=\frac{32\pi\alpha_s(Q)}{9m^2}(1-x)\ . \tag{21}$$

Note that x is a constant which depends on the quark mass m and the scale factor μ. Because μ is appreciably less than m [5], x is positive. Now we can take the Fourier transform of $y(Q)$, obtaining

$$Y_1(r)=(2/3m^2)(1-x)\nabla^2V(r)=Y_{\rm GFB}(r)(1-x)\ , \tag{22}$$

where $Y_1(r)$ is the value of $Y(r)$ using our approximation (1). In this approximation, we have reduced the interaction to the form of the GFB interaction except that it is multiplied by the constant $1-x$.

Because (7) holds, the sign of $\langle Y_1(r)\rangle$ is the same as the sign of $1-x$. In the S state, we must have $x<1$, or the sign of the S-wave color-hyperfine splitting will disagree with experiment. If the value of the scale μ is not too different in S and P states, then this approximation leads us to the conclusion that

$$\Delta M_{1Ph}=(1-x)\Delta M_{Ph}(\mathrm{GFB})>0\ . \tag{23}$$

If x lies in the range $0<x<1$, then ΔM_{1Ph} is positive, but smaller in magnitude than the value obtained in the GFB approximation.

We now discuss the scale μ, which in general is different in P and S states. The reason is that a P-state wave function is more spread out in r space than an S-state wave function, and so in Q space the P-wave function has its main support nearer the origin. Therefore, in our approximation of replacing $\alpha_s(Q)$ by $\alpha_s(\mu)$, the appropriate value of μ is smaller in the P state than in the S state. This has the effect of making x larger in the P state than in the S state. Therefore, if we use a value of x appropriate to the S state, we overestimate the value of ΔM_{Ph}. In this way we can get an upper limit on ΔM_{Ph} from Eq. (23).

(2) In our second method, we begin by approximating $\alpha_s(Q)$ within the square brackets in Eq. (11) by $\alpha_s(\mu)$. We then make use of Eqs. (18) and (20) and rearrange terms to obtain

$$y(Q)=\frac{32\pi\alpha_s(Q)}{9m^2}\left[1-x-\frac{63}{2(33-2n_f)}\right]+\frac{112\pi\alpha_s(\mu)}{(33-2n_f)m^2}\ . \tag{24}$$

Taking the Fourier transform and using Eq. (4), we get

$$Y_2(r)=Y_{\rm GFB}(r)\left[1-x-\frac{63}{2(33-2n_f)}\right]+\frac{112\pi\alpha_s(\mu)}{(33-2n_f)m^2}\delta(\mathbf{r}) , \quad (25)$$

where $Y_2(r)$ is the value of $Y(r)$ using our approximation (2). The last term in Eq. (25), although positive, does not contribute to ΔM_{2Ph} because the expectation value of a δ function vanishes in P states. We then obtain the following expression for ΔM_{2Ph}:

$$\Delta M_{2Ph}=\left[1-x-\frac{63}{2(33-2n_f)}\right]\Delta M_{Ph}(\mathrm{GFB}) . \quad (26)$$

We see that Eq. (28) is quite different from Eq. (24). Making use of our previous observation that $x>0$, we see that in our second approximation the sign of ΔM_{Ph} is negative, just as the one-loop calculations with both powers of α_s fixed. If we had not made the approximations of this second method, the δ function in Eq. (25) would have been smeared out, and we would have obtained an additional positive contribution to ΔM_{Ph}. Therefore, we believe that our second method underestimates the value of ΔM_{Ph}.

We next consider in more detail the question of the appropriate values of μ. Here we are guided by the work of Pantaleone *et al.* [5], who have used experimental data to estimate values of μ for the S-wave color-hyperfine interaction in charmonium and for the P-wave tensor interaction in both charmonium and bottomonium. To obtain an upper limit, we should use the S-wave values of μ in Eq. (23), while to obtain a lower limit, we should use the P-wave values in Eq. (26).

Pantaleone *et al.* [5] estimate that the value of μ relevant to the S-wave color-hyperfine interaction in charmonium is in the range $0.77<\mu<1.25$ GeV, depending on the potential and on their prescription. For bottomonium, unfortunately, the S-wave color-hyperfine splitting is not known, so the value of μ is not given in this case. The values of μ in P states can be given for the tensor interaction. Pantaleone *et al.* [5] estimate that the values of μ are in the range $0.52<\mu<0.68$ GeV for charmonium and in the range $1.2<\mu<1.5$ GeV for bottomonium. Using the mean values of these estimates, we obtain $\mu=1.0$ GeV and $\mu=0.6$ GeV, respectively, for the upper and lower limits in charmonium. For bottomonium, we use the mean value $\mu=1.35$ GeV for the lower limit, and make the reasonable guess $\mu=2$ GeV (a little larger than the P-state values found by Pantaleone *et al.*) for the upper limit.

We use the $\overline{\rm MS}$ scheme to obtain $\alpha_s(\mu)$ for the various values of μ. Using $m_c=1.65$ GeV, $m_b=5.0$ GeV, and $n_f=3$ for $\mu\le m_c$, $n_f=4$ for $\mu>m_c$, we can calculate x. We obtain for charmonium

$$x(\mu=1.0)=0.30, \quad x(\mu=0.6)=1.14 , \quad (27)$$

and for bottomonium

$$x(\mu=1.35)=0.61, \quad x(\mu=2.0)=0.39 . \quad (28)$$

In each case we use the smaller value of x in Eq. (23) to get an upper limit on the splitting, and the larger value of x in Eq. (26) to get a lower limit. This is a conservative approach in that it leads to a larger difference between the upper and lower limits than using the same values of μ in Eqs. (23) and (26).

In order to make use of Eqs. (23) and (26), we need an estimate of $\Delta M_{Ph}(\mathrm{GFB})$. This quantity has been calculated in Ref. [1] for the $1P$ state in charmonium and the $1P$ and $2P$ states in bottomonium. The result in charmonium is $\Delta M_{Ph}(\mathrm{GFB})=4.1$ MeV. In the bottomonium $1P$ and $2P$ states the results are $\Delta M_{Ph}(\mathrm{GFB})=1.7$ MeV, $\Delta M_{Ph}(\mathrm{GFB})=1.2$ MeV, respectively. Although the calculation in Ref. [1] is model dependent, the results are useful for giving us reasonable estimates. We obtain

$$\begin{aligned} -5.4\ \mathrm{MeV} &\lesssim \Delta M_{Ph}(1\ \bar{c}c) \lesssim 2.9\ \mathrm{MeV} , \\ -1.3\ \mathrm{MeV} &\lesssim \Delta M_{Ph}(1\ \bar{b}b) \lesssim 1.0\ \mathrm{MeV} , \\ -0.9\ \mathrm{MeV} &\lesssim \Delta M_{Ph}(2\ \bar{b}b) \lesssim 0.7\ \mathrm{MeV} . \end{aligned} \quad (29)$$

These limits are not really firm because they depend on our taking "reasonable" values of μ as well as model-dependent values of $\Delta M_{Ph}(\mathrm{GFB})$. We also do not know the effect of the two-loop terms we have omitted. Nevertheless, because we have been so conservative in the formulas used for estimating our limits, we believe that the values of ΔM_{Ph} for charmonium and bottomonium are likely to lie in the intervals given in Eq. (29).

We emphasize that we have addressed the question of the splitting arising from the QCD color-hyperfine interaction. There are other contributions to ΔM_P which we have omitted. For example, if we do not treat the tensor and spin-orbit forces as small perturbations, their effects do not cancel out of the center of mass of the ^3P levels. As another example, the coupling of a level to decay channels not only gives the level a width, but also in general changes the energy. As a third example, if the confining part of the potential does not transform as a Lorentz scalar, as we have implicitly assumed [18], but contains a part that transforms like the time component of a four-vector, the vector part will contribute to ΔM_P. Because of the possible existence of these and perhaps still other contributions to ΔM_P, it would be rash to say that the major contribution is from the color-hyperfine interaction when the splitting arising from that interaction is so small.

Very recently, we learned of a preliminary measurement of the mass of the $^1P_1$ state of charmonium in E760 at Fermilab [19], which yields $\Delta M_P\simeq -1$ MeV. This result lies well within the limits given in Eq. (29).

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