Re-study of the contribution of scalar potential and spectra of $c\bar{c}$, $b\bar{b}$ and $b\bar{c}(\bar{b}c)$ families*

YUAN Xu-Hao(袁煦昊)[1;1)] KE Hong-Wei(柯红卫)[2;2)]
DING Yi-Bing(丁亦兵)[3] LI Xue-Qian(李学潜)[1;3)]

[1] School of Physics, Nankai University, Tianjin 300071, China
[2] School of Science, Tianjin University, Tianjin 300072, China
[3] College of Physics Sciences, Graduate University of Chinese Academy of Sciences, Beijing 100049, China

Abstract: We indicated in our previous work that for QED the role of the scalar potential which appears at the loop level is much smaller than that of the vector potential and is in fact negligible. But the situation is different for QCD, one reason is that the loop effects are more significant because α_s is much larger than α, and second the non-perturbative QCD effects may induce a sizable scalar potential. In this work, we study phenomenologically the contribution of the scalar potential to the spectra of charmonia, bottomonia and $b\bar{c}(\bar{b}c)$ families. Taking into account both vector and scalar potentials, by fitting the well measured charmonia and bottomonia spectra, we re-fix the relevant parameters and test them by calculating other states of not only the charmonia and bottomonia families, but also the $b\bar{c}$ family. We also consider the Lamb shift of the spectra.

Key words: charmonia, bottomonia, scalar potential, Lamb shift

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1 Introduction

The potential model has been proposed to evaluate the spectra of the quantum systems composed of heavy flavors, such as charmonia and bottomonia for many years [1]. The subject on heavy quarkonia was thoroughly discussed in an enlightening paper [2]. Even though one calculates the binding energy in terms of the non-relativistic Schrödinger equation, it is indeed a reasonable framework for such heavy resonant states. The main physics, despite being induced by the standard model (SM) or new physics beyond the SM, is included in the potential. In phenomenology, the potential contains two pieces, the Coulomb potential, which is induced by the gluon exchange, and confinement, which may come from non-perturbative QCD effects or other sources. It was suggested that due to the symmetry consideration [3], of the QED case, if the Dirac equation has a higher degree of symmetry than the corresponding Schrödinger equation, the Coulomb potential should have both scalar and vector parts with equal fractions. However, for such a combination the hydrogen potential would not possess the coupling of orbital angular momentum and spin ($L\cdot S$) and it definitely contradicts the reality.

In our previous work [4], we analyzed the source of the scalar and vector potentials for the QED, namely the vector potential is induced by a one-photon exchange for the vector-like gauge theory QED, while the scalar part must come from the loop effects. Therefore, for the QED case, the fraction of the scalar potential is suppressed because the coupling $\alpha\sim 1/137$ is small and does not have a substantial contribution to the spectrum of hydrogen. This conclusion is consistent with the precise measurement

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1) E-mail: segoat@mail.nankai.edu.cn
2) E-mail: khw020056@hotmail.com, corresponding author
3) E-mail: lixq@nankai.edu.cn

of the spectra of hydrogen-like atoms. However, for the QCD case, the situation is very different. First, because the strong coupling $\alpha_{\rm s}$ is much larger than α, loop suppression is not as great as for the QED and sometimes the NLO effect of QCD can even exceed the leading order [5, 6]. Second, non-perturbative effects may also change the whole scenario. Thus for QCD, the scalar potential may play an important role and its contribution may especially manifest at values of the spectrum line splitting due to the coupling of orbital angular momentum and spin. That was also suggested by other authors [7].

Because non-perturbative QCD effects cannot be reliably derived from any underlying theory so far, we prefer to introduce phenomenological parameters to manifest their roles and the parameters are fixed by fitting the well-measured data. Indeed the parameters contain the contribution not only of non-perturbative effects, but also of higher orders of perturbative effects. In our last work [8], we introduced two more parameters to account for the scalar piece in the potential and then re-fitted the spectra of charmonia. The fitting is much improved compared with that including only the vector piece. Thus for further investigating the involvement of scalar potential, we use the same strategy adopted in Ref. [8] to evaluate the spectra of the bottomonia ($\rm b\bar{b}$) and then the various resonant states of the $\rm b\bar{c}(\bar{b}c)$ system. Namely, we write $U(r)=V(r)+S(r)$ and the vector potential is $V(r)=-c\ C_{\rm F}\alpha_{\rm s}/r+d\kappa^2 r$, while the scalar one is $S(r)=-(a-c)C_{\rm F}\alpha_{\rm s}/r+(b-d)\kappa^2 r$ with a, b, c, d four parameters to be determined. The induced terms, such as $L\cdot S$ coupling, $S_1\cdot S_2$ coupling and the spin-independent corrections, etc. are given in very enlightening work by Lucha et al. [9–11]. Substituting all the expressions into the Schrödinger equation, we may obtain the spectra of heavy quark-antiquark systems.

In addition, QED theory predicts the Lamb shift which is due to vacuum effects. In QM, it only shifts the S-wave spectra because in the non-relativistic limit, it is proportional to $\delta(\boldsymbol{r})$, but by the quantum field theory, the $L\neq 0$ states are also affected. In other words, by considering the Lamb shift, the positions of the spectra would deviate from those obtained without the Lamb shift. For the hadron case, the governing theory is QCD which also induces the Lamb shift [12], and in this work, we include its contribution. It is noted that, as the phenomenological parameters (which are determined by fitting data) are introduced, all higher order effects should also be automatically involved, so it seems that there is no need to consider Lamb shifts, which are induced by the loop effects. In fact, there is. However, as calculating the form factors of the hadronic transition matrix elements or obtaining the parton distribution functions, we always wish to squeeze the uncontrollable parts that are not calculable, such as the non-perturbative contributions, to be as small as possible. Similarly, here we include the NLO or even NNLO corrections i.e, the Lamb shifts and re-fit the parameters which are indeed not derivable.

Considering the Lamb shift, there is a byproduct that may be very helpful in understanding the theory. Obviously, only the products $c\alpha_{\rm s}$ and $d\kappa^2$ in the potential matter, but not c, d, $\alpha_{\rm s}$ and κ separately. However, for explicitly showing the roles of the scalar and vector pieces, we adopt a special strategy.

When the Lamb shift is taken into account, the situation may change slightly. In the expression of the Lamb shift, there is an ultraviolet divergent term which includes the renormalization scale μ. Meanwhile the running coupling $\alpha_{\rm s}$ also depends on the scale. The authors of [13, 14] suggest an effective method to deal with divergence and meanwhile fix the value of $\alpha_{\rm s}$ (see the text, where we introduce the method in some detail for the readers' convenience). It is noted that μ is a complicated function of $\alpha_{\rm s}$, quark mass ($m_{\rm b}$ or $m_{\rm c}$), and the principal quantum number n. Taking a special way to determine μ which corresponds to adopting a special renormalization scheme, and considering the dependence of $\alpha_{\rm s}$ on μ, one can eventually find the value of $\alpha_{\rm s}$ for a certain flavor (b or c) and a given principal quantum number. For example, for $\Upsilon(1S)$, we have $\alpha_{\rm s}=0.284$ for $m_{\rm b}=4.8$ GeV and the scale-parameter $\Lambda=0.2$ GeV. Amazingly, this value is quite close to that adopted in literature by fitting the Υ spectra.

By contrast, the confinement term κr comes from the non-perturbative QCD effects and cannot be theoretically derived so far. Thus we adopt the value given in Ref. [15].

With all the inputs, we calculate the spectra of the $\rm c\bar{c}$, $\rm b\bar{b}$ and $\rm \bar{b}c(b\bar{c})$ systems.

This paper is organized as follows. In Section 2 and 3, we introduce the generalized Breit-Fermi Hamiltonian and the Schrödinger equation for the $\rm b\bar{b}$ bound states: $\Upsilon(1S)$, $\chi_{\rm b0}(1P)$, $\chi_{\rm b1}(1P)$, $\chi_{\rm b2}(1P)$ and $\Upsilon(2S)$. Then we numerically solve the eigenequations for these bound states and fix the parameters as we did for dealing with the charmonia family in our previous work. In Section 4, the Lamb shift is taken into account and another set of the parameters is given to improve our predictions. In Section 5,

we give the spectra of the $\bar{b}c(b\bar{c})$ mesons. The last section is devoted to our conclusion and discussion.

2 The generalized Breit-Fermi Hamiltonian and Schördinger equation

The generalized Breit-Fermi Hamiltonian was given in Refs. [9–11] as

$$H = H_0 + H_1 + \dots , \tag{1a}$$

$$H_0 = \frac{p^2}{m} + 2m + S(r) + V(r) , \tag{1b}$$

$$H_1 = H_{\rm sd} + H_{\rm si} , \tag{1c}$$

$$\begin{aligned} H_{\rm sd} &= H_{\rm ls} + H_{\rm ss} + H_{\rm t} \\ &= \frac{1}{2m^2 r}(3V' - S')\, L\cdot(S_1+S_2) + \frac{2}{3m^2} S_1\cdot S_2 \\ &\quad \times\nabla^2 V(r) + \frac{1}{12m^2}\left(\frac{1}{r}V' - V''\right) S_{12}, \end{aligned} \tag{1d}$$

$$\begin{aligned} H_{\rm si} &= -\frac{p^4}{4m^3} + \frac{1}{4m^2}\left\{\frac{2}{r}V'(r)\cdot L^2 + [p^2, V - rV']\right. \\ &\quad \left. + 2(V - rV')p^2 + \frac{1}{2}\left[\frac{8}{r}V'(r) + V'' - rV'''\right]\right\}, \end{aligned} \tag{1e}$$

where, V and S stand for the vector and scalar potentials and $H_{\rm si}$ and $H_{\rm sd}$ represent the spin-independent and spin-dependent pieces respectively. For the linear confinement piece we adopt the Cornell potential [16]. Thus the total potential at the lowest order reads

$$U(r) = V(r) + S(r) = -aC_{\rm F}\frac{\alpha_{\rm s}}{r} + b\kappa^2 r, \tag{2a}$$

where

$$\begin{cases} V(r) = -c\ C_{\rm F}\alpha_{\rm s}/r + d\kappa^2 r \\ S(r) = -(a-c)C_{\rm F}\alpha_{\rm s}/r + (b-d)\kappa^2 r \end{cases} . \tag{2b}$$

With the Hamiltonian (1) and the potential (2), one can solve the Schrödinger equation

$$H\Psi(r) = (H_0 + H_1)\Psi(r) = (E + 2m)\Psi(r). \tag{3}$$

We can transform the radial wave function into $R(x)$ with a dimensionless variable: $x = \kappa r$, then the reduced radial equation is written as[1)]

$$\frac{{\rm d}^2}{{\rm d}x^2}u(x) = A(x)u(x), \tag{4a}$$

where,

$$\begin{aligned} A(x) &= -\tilde{m}\left(\tilde{E} - \tilde{U}(x) - \tilde{H}_1'\right) + \frac{l(l+1)}{x^2} \\ &\quad -\frac{1}{4}\left(\tilde{E} - \tilde{U}(x)\right)^2, \end{aligned} \tag{4b}$$

$$\begin{cases} \tilde{m} = m/\kappa, \quad \tilde{E} = E/\kappa, \\ \tilde{H}_1' = H_1'/\kappa,\ \tilde{U}(x) = U(x)/\kappa, \end{cases} \tag{4c}$$

and

$$H_1 = H_1' - \frac{p^4}{4m^3}. \tag{4d}$$

In the simplified potential form (3), the approximation

$$p^4 \sim \left[m\,(E - U(r))\right]^2 \tag{4e}$$

is used. The legitimacy of applying this approximation to the calculation and the error degree brought up in the numerical values are briefly discussed in the appendix.

It is noted that the $1/r^3$ and $\delta(r)$ terms are rather singular and their existence seem to cause uncertainties in the theoretical predictions. In fact, this problem also exists in the calculation of the hydrogen atom spectra, but it is benign. The reason is that we note that the $1/r^3$ terms are associated with the $L-S$ coupling proportional to $\frac{1}{r^3}L\cdot S$ which is zero for the $l=0$ S-wave, and the first non-zero terms are the P-wave whose radial wavefunction is proportional to r, whereas the radial wavefunctions of the states are proportional to r^l. With the perturbation method, one sandwiches these terms between eigen-functions which are obtained by the Schrödinger equation without such terms, thus for the the P-wave, the $1/r^3$ and $\delta(r)$ singularities are smeared out in the integration. We also showed in our earlier studies [19] that singularities do not affect the stability of solutions when a variational method is employed. In this work, the Hamiltonian includes not only the Coulomb piece, but also the confinement one, the solution is no longer analytical as for the hydrogen-like atoms, but the small-r behavior of the solution should be determined by the Coulomb potential and the argument for the hydrogen case can be generalized here. As we definitely know that such singularities are benign, when we carry out integrations, we deliberately set a lower boundary for r_0 (for compromising the computer), and when we vary the value of r_0, we find that the results are indeed stable. Thus we confirm that

1) The standard form of the radial equation can be easily found in Ref. [17], and the method to make it dimensionless is borrowed from Ref. [18].

the existence of such superficial singularities does not affect the reliability of our theoretical predictions.

3 The energy gap Function for The $b\bar{b}$ bottomonia and the numerical results without taking into account the Lamb shift

The radial equation (4) can be solved in terms of a method called "the iterative numerical process" which is introduced in the literature (for example, see Refs. [17, 18]). We have improved this method, and then fix the parameters a, b, c, d by fitting the well-measured spectra of bottomonia. In our previous work [8], we explain the reason for the choice of the input for charmonia. However, for bottomonia, the situation is slightly different and the masses of $\Upsilon(1S)$, $\chi_{\rm b0}(1P)$, $\chi_{\rm b1}(1P)$, $\chi_{\rm b2}(1P)$ and $\Upsilon(2S)$ are chosen for obtaining the values of a, b, c and d. Similar to the procedure used in our previous work [8], instead of directly fitting the masses, we construct a series of relations which should be fitted:

$$\begin{cases} m[\Upsilon(2S)]-m[\Upsilon(1S)]=E[2^3S_1]-E[1^3S_1]; \\ m[\Upsilon(2S)]-m[\chi_{\rm b0}(1P)]=E[2^3S_1]-E[1^3P_0]; \\ m[\Upsilon(2S)]-m[\chi_{\rm b1}(1P)]=E[2^3S_1]-E[1^3P_1]; \\ m[\Upsilon(2S)]-m[\chi_{\rm b2}(1P)]=E[2^3S_1]-E[1^3P_2]\ , \end{cases} \quad (5)$$

where, $E[n_r^{2s+1}l_j]$ represents the eigen-values of the radial equations (4) with various quantum numbers n_r, j, l, and s for the bottomonia. Because the parameters a, b, c and d are involved in the potential (2), $E[n_r^{2s+1}l_j]$ must be functions of these parameters. m[meson] are the masses of the individual states which are shown in the following Table 1 [20]. Sequentially, the parameters a, b, c and d are obtained by solving Eqs. (5). By employing Newton's iterative method (The details of the numerical method can be found in Ref. [21].), we have achieved:

$$a=1.2165,\ b=1.2988,\ c=0.8686,\ d=0.5886. \quad (6)$$

Here we set $\alpha_{\rm s}=0.284$ and $\kappa=0.42$ GeV which seem somehow different from the values given in the literature [15, 22, 23]. But as noted, the deviation may be included in the phenomenological parameters a, b, c and d. The choice of $\alpha_{\rm s}$ has another reason which is associated with our treatment of the contribution of the Lamb shift (see next section), and this value is not very far from that given in the literature. Given a, b, c and d in (6), the masses of the bottomonia states are determined as:

$$M(n_r^{2s+1}l_j)=E[n_r^{2s+1}l_j]+E_0, \quad (7)$$

where, E_0 is the zero-point energy:

$$E_0=m[\Upsilon(1S)]-E[1^3S_1] \quad (8)$$

and the final results are shown in Table 1 below.

Explicitly, in the process, the masses of the mesons with superscript "fit" are taken as inputs to obtain the parameters and then the masses of other states in the table are predicted.

For readers' convenience and to give a clear comparison, we also list the results for the charmonia which were obtained in our previous work [8] with

$$a=1.1715,\ b=1.2250,\ c=0.8087,\ d=0.5291, \quad (9)$$

in Table 2[1)].

Table 1. The mass spectra for the bottomonia states (in GeV), with $m_{\rm b}=4.8$ GeV. The $M_{\rm EXP}$ is the value of the mass given in PDG [20].

meson	$M_{\rm EXP}$	prediction	meson	$M_{\rm EXP}$	prediction	meson	$M_{\rm EXP}$	prediction
$\eta_{\rm b}(1^1S_0)$	9.3909	9.4124	$h_{\rm b}(1^1P_1)$		9.8897	$\Upsilon(1^3D_1)$	10.1611	10.1607
$\Upsilon(1^3S_1)^{\rm fit}$	9.4603	9.4603	$\chi_{\rm b2}(1^3P_2)^{\rm fit}$	9.9122	9.9122	$\Upsilon(1^3D_2)$		10.1719
$\chi_{\rm b0}(1^3P_0)^{\rm fit}$	9.8594	9.8594	$\eta_{\rm b}(2^1S_0)$		9.9932	$\Upsilon(1^3D_3)$		10.1827
$\chi_{\rm b1}(1^3P_1)^{\rm fit}$	9.8928	9.8928	$\Upsilon(2^3S_1)^{\rm fit}$	10.0233	10.0233	$\Upsilon(3^3S_1)$	10.3552	10.3949

Table 2. The mass spectra for the charmonia states (in GeV), with $m_{\rm c}=1.84$ GeV. $M_{\rm EXP}$ is the value of the mass given in PDG [20], $M_{\rm a}$ is the prediction with 4 parameters, and $M_{\rm b}$ is the prediction with 3 parameters.

meson	$M_{\rm EXP}$	$M_{\rm a}$	$M_{\rm b}$	meson	$M_{\rm EXP}$	$M_{\rm a}$	$M_{\rm b}$
$\eta_{\rm c}(1^1S_0)$	2.9803	$3.0189^{+0.0019}_{-0.0026}$	$3.0290^{+0.0003}_{-0.0006}$	$\chi_{\rm c2}(1^3P_2)$	3.5562	$3.5564^{+0.0007}_{-0.0003}$	$3.5324^{+0.0013}_{-0.0008}$
$J/\psi(1^3S_1)$	3.0969	$3.0969^{\rm fit}$	$3.0969^{\rm fit}$	$\eta_{\rm c}(2^1S_0)$	3.6370	$3.6370^{\rm fit}$	$3.6227^{+0.0027}_{-0.0019}$
$\chi_{\rm c0}(1^3P_0)$	3.4148	$3.4148^{\rm fit}$	$3.4148^{\rm fit}$	$\psi(2^3S_1)$	3.6861	$3.6861^{\rm fit}$	$3.6861^{\rm fit}$
$\chi_{\rm c1}(1^3P_1)$	3.5107	$3.5107^{\rm fit}$	$3.5107^{\rm fit}$	$\psi(3^3{\rm S}_1)$		$4.1164^{+0.0083}_{-0.0071}$	$4.1194^{+0.0126}_{-0.0107}$
$h_{\rm c}(1^1P_1)$	3.5259	$3.5100^{+0.0031}_{-0.0025}$	$3.4849^{+0.0030}_{-0.0027}$				

1) The errors in our numerical computations come from the inputs, namely the uncertainties of the experimental data.

By fitting the earlier data, the authors of Refs. [10] and [24] suggested that the confining potential be scalar, which requires the parameter d in our work to be zero. By fitting the up-to-date experimental results, we may reach different conclusions. Here we take another scheme where the parameter set of only a, b and c is adopted, the masses of the J/ψ, χ_{c0}, χ_{c1} and $\psi(2S)$ as the inputs, we obtain the parameters as:

$$a=1.1061,\ b=1.2235,\ c=1.0135, \tag{10}$$

with $\alpha_s=0.36$ and $\kappa=0.42$. We list the predictions on the mass spectra of the rest states of charmonia in the Table 2 where subscript a refers to the scheme with the four-parameter set and b for the scheme with the three-parameter set. From Table 2, it is clear that the predictions with the four-parameter set are better than those obtained with the 3-parameter set.

On the other hand, some authors still suggested that the confinement potential be a sum of vector and scalar parts (see Ref. [25]). Therefore, in our work, we choose the scheme with $d\neq 0$ to make predictions on the spectra of $b\bar{c}(c\bar{b})$ systems.

4 The mass spectra of the bottomonia as the Lamb shift is taken into account

As is well known, the Lamb shift is due to vacuum fluctuation and may cause sizable effects on the meson spectra. Indeed, the QED Lamb shift may not be very significant because of the smallness of the fine structure constant α [26], in fact, it just reaches the order of 10^{-7} eV, but for the QCD case, the situation is different.

In the previous section the effects of the Lamb shift are not included in the eigen-energy (4). Thus in this section, we take the Lamb shift into account. However, we do not introduce the Hamiltonian induced by the Lamb shift into the differential equation because the corresponding pieces are very complicated. Instead, according to the traditional method, we calculate the effects in terms of wavefunctions obtained with the original Hamiltonian, i.e. accounting $\langle\Psi|H_{\rm Lamb}|\Psi\rangle$, where $H_{\rm Lamb}$ is obtained via the loop diagrams and simply add the estimated values into the binding energies of various states. Including the Lamb shift effects in the expressions of the spectra, we re-fit the data to obtain the parameters a, b, c and d again and predict the mass spectra of the rest resonances.

Namely, we set the masses of the bound states to be the measured values:

$$2m_b+E+\Delta E_{\rm LM}=M_{\rm EXP}, \tag{11}$$

where E is the solution of the eigen-equation, $\Delta E_{\rm LM}$ is the energy caused by the Lamb shift and $M_{\rm EXP}$ has been defined in Tables 1 and 2 already. Solving the equation, one can obtain the parameters again.

The authors of Refs. [12–14] gave the theoretical expressions for the binding energies which involve contributions of the Lamb shift. It is well known that the induced Hamiltonian contributing to the Lamb shift is due to the vacuum fluctuation and can be obtained by calculating the loop diagrams order by order. Thus the Lamb Shift starts at $O(\alpha_s^2)$ [13][1)]. The Lamb shift is:

$$\Delta E_{\rm LM}=\langle\Psi|V_{\rm Lamb}|\Psi\rangle,$$

where Ψ is the solution of the Schrödinger equation containing only the Coulomb piece, which can be written as :

$$\Delta E_{\rm LM}[n,j,l,s]=m\Big[\Delta E(\alpha_s^3)+\Delta E(\alpha_s^4)+\Delta E(\alpha_s^5)+\Delta E(\alpha_s^6)+\cdots\Big]. \tag{12a}$$

For illustrating the contribution of the Lamb shift to the spectra, let us directly copy Titard's formulas [13] below, where we dropped the tree-level terms and the relativistic corrections, and we have:

$$\Delta E(\alpha_s^3)=-\alpha_s^3\frac{C_F^2}{8\pi n^2}(2\beta_0\gamma_E+4a_1); \tag{12b}$$

$$\Delta E(\alpha_s^4)=-\alpha_s^4\frac{C_F^2}{4n^2\pi^2}\left\{\left(a_1+\gamma_E\frac{\beta_0}{2}\right)^2+2\left[\gamma_E\left(a_1\beta_0+\frac{\beta_1}{8}\right)+\left(\frac{\pi^2}{12}+\gamma_E^2\right)\frac{\beta_0^2}{4}+b_1\right]\right\}, \tag{12c}$$

where, n in Eq. (12) stands for the principal quantum number as $n=n_r+l$, where, n_r and l are defined in

1) We indicate that the Lamb shift effects start from $O(\alpha_s^2)$, and it seems that this allegation conflicts with Eq. (12). As noted, in the expression Eq. (12) which is given in Ref. [13], $\Delta E_{\rm LM}$ is not the potential derived from the loop, but the expectation value of the potential with the wavefunctions which are solutions of the Schrödinger equation containing only the Coulomb piece. Since such solutions possess an exponential factor $\exp(-\alpha_s\mu r)$, the expectation value of any function of r as $f(r)$ should be proportional to α_s^n ($n\geqslant 1$), thus the $\Delta E_{\rm LM}$ in Eq. (11) start from α_s^3. But indeed the potential pieces corresponding to the Lamb shifts directly come from the loop diagrams which start from $O(\alpha_s^2)$.

Section 3. All the constants as a_1, a_2, b_1, β_i $(i=1,2,3)$ are given in Ref. [27] (also see Refs. [13, 28–31]). Furthermore, Hoang et al. estimated the contribution of higher orders up to $O(\alpha_{\rm s}^5)$ and $O(\alpha_{\rm s}^6)$ to the binding energies (See Ref. [12]).

When we calculate the QCD Lamb shift effects for the hadron spectra, the potential not only contains the Coulomb piece, but also the confinement, so that the expression would be more complicated than that shown in Eqs. (11b) and (11c). In fact, there cannot be analytical expressions for the expectation values.

The Lamb shift $\Delta E_{\rm LM}$ $[n,\ j,\ l,\ s]$ depends on the coupling constant $\alpha_{\rm s}$ in Eq. (12) as [13]:

$$\alpha_{\rm s}(\mu^2) = \frac{2\pi}{\beta_0 \ln \mu/\Lambda}\Bigg\{1-\frac{\beta_1}{\beta_0^2}\frac{\ln(\ln\mu^2/\Lambda^2)}{\ln\mu^2/\Lambda^2} + \frac{1}{\beta_0^4 \ln^2\mu^2/\Lambda^2}\Big[\beta_1^2\ln^2(\ln\mu^2/\Lambda^2) - \beta_1^2\ln(\ln\mu^2/\Lambda^2) - \beta_1^2+\beta_2\beta_0\Big]\Bigg\}. \quad (13)$$

Using the formulas given above, one can evaluate the Lamb shift of the charmonia states. The choice of the renormalization point μ is suggested by Pineda et al., and "a natural value for this parameter" is [13, 27]:

$$\mu = \frac{2}{n a_{\rm B}}, \quad (14a)$$

where,

$$a_{\rm B} = \frac{2}{m C_{\rm F}\tilde{a}_{\rm s}}, \quad (14b)$$

$$\tilde{\alpha}_{\rm s}(\mu^2) = \alpha_{\rm s}\Bigg\{1+\left(a_1+\frac{\gamma_{\rm E}\beta_0}{2}\right)\frac{\alpha_{\rm s}}{\pi}\Bigg[\gamma_{\rm E}\left(a_1\beta_0+\frac{\beta_1}{8}\right) + \left(\frac{\pi^2}{12}+\gamma_{\rm E}^2\right)\frac{\beta_0^2}{4}+b_1\Bigg]\frac{\alpha_{\rm s}^2}{\pi^2}\Bigg\}. \quad (14c)$$

In the expression of the newly derived Hamiltonian there is a term $\ln 2\alpha\mu r/r$ (after a Fourier transformation from the momentum space to the configuration space), which is UV divergent. To deal with the divergence, it is suggested to take an effective method. For a smaller range of r the Coulomb piece $1/r$ obviously dominates, so in $\langle\Psi|H_{\rm Lamb}|\Psi\rangle$ one can use the wavefunction Ψ which is the solution of the Schrödinger equation containing only the Coulomb potential, namely we can have an analytical solution for this asymptotic situation. Thus $\langle\Psi|\ln 2\alpha\mu r/r|\Psi\rangle \propto \ln(na\mu/2)$. To make the UV divergence vanish, the suggested renormalization scheme is to set $\mu = 2/na_{\rm B}$. Indeed, in Ref. [13], three other alternative schemes were also suggested, here we just take this one and find that the value of $\alpha_{\rm s}$ determined with this scheme is closer to that adopted in early literature for calculating the spectra of bottomonia.

The value of the parameter Λ is chosen as 0.2 GeV for bottomonia [27], and at this point,

$$\alpha_{\rm s}^{n=2} = 0.284, \quad (15)$$

which is the value of $\alpha_{\rm s}$ we used in Section 3. It is noted that $\alpha_{\rm s}$ is different for different a quantum number n:

$$\alpha_{\rm s}^{n=1} = 0.24\ ,\ \alpha_{\rm s}^{n=2} = 0.284,\ \alpha_{\rm s}^{n=3} = 0.316. \quad (16)$$

We will use the n-related $\alpha_{\rm s}$ value for evaluating the spectra of the radially excited states of bottomonia.

Simply adding the Lamb shift to the total binding energy is like our change of the zero-point energy for each state. We still select masses of $\Upsilon(1S)$, $\chi_{\rm b0}(1P)$, $\chi_{\rm b1}(1P)$, $\chi_{\rm b2}(1P)$, $\Upsilon(2S)$ as inputs, and solve the equation (5) again as we did in last section. But the value of $\alpha_{\rm s}$ in (5) is taken as that given in Eq. (16) which depends on n. The new solutions of a, b, c and d are:

$$a^{\rm (LM)} = 1.4256,\ b^{\rm (LM)} = 1.3553, \quad c^{\rm (LM)} = 0.8077,\ d^{\rm (LM)} = 0.6849, \quad (17)$$

where the superscript LM refers to all the corresponding parameters obtained as the Lamb shift is taken into account.

With these solutions, our predictions on the whole family spectra of bottomonia are presented in Table 3.

Table 3. The mass spectra with the Lamb shift (in GeV), where, the LM stands for the contribution of the Lamb shift, M is the predicted mass when the parameters are set as in Eq. (17) and M' stands for $M' = M + \Delta E_{\rm LM}$.

meson	$\Delta E_{\rm LM}$	M	M'	$M_{\rm EXP}$	meson	$\Delta E_{\rm LM}$	M	M'	$M_{\rm EXP}$
$\eta_{\rm b}(1^1S_0)$	−0.1064	9.5274	9.4210	9.3020	$\eta_{\rm b}(2^1S_0)$	−0.0549	10.0451	9.9902	
$\Upsilon(1^3S_1)^{\rm fit}$	−0.1114	9.5717	9.4603	9.4603	$\Upsilon(2^3S_1)^{\rm fit}$	−0.0561	10.0794	10.0233	10.0233
$\chi_{\rm b0}(1^3P_0)^{\rm fit}$	−0.0618	9.9212	9.8594	9.8594	$\Upsilon(1^3D_1)$	−0.0412	10.2139	10.1727	10.1611
$\chi_{\rm b1}(1^3P_1)^{\rm fit}$	−0.0620	9.9548	9.8928	9.8928	$\Upsilon(1^3{\rm D}_2)$	−0.0412	10.2272	10.1860	
$\rm h_b(1^1P_1)$	−0.0621	9.9507	9.8887		$\Upsilon(1^3D_3)$	−0.0412	10.2399	10.1987	
$\chi_{\rm b2}(1^3P_2)^{\rm fit}$	−0.0622	9.9744	9.9122	9.9122	$\Upsilon(3^3S_1)$	−0.0379	10.4380	10.4001	10.3552

5 The spectra of the $b\bar{c}(\bar{b}c)$ mesons

In this section, we study further the spectra of the $b\bar{c}(\bar{b}c)$ mesons. Except for the ground state B_c, the other states of the $b\bar{c}$ mesons have not been well measured yet [20], so we cannot directly fit the parameters from data as we do for charmonia and bottomonia. It is noted that the parameters for charmonia and bottomonia are not drastically different and since the $b\bar{c}(\bar{b}c)$ family lies between charmonia and bottomonia, we may interpolate those parameters for the $b\bar{c}(\bar{b}c)$ family, namely average the values for charmonia and botomonia to be that for $b\bar{c}(\bar{b}c)$ mesons (See Table 4).

Table 4. The parameters for $b\bar{c}$ (or $\bar{b}c$) mesons, where the parameters of charmonia can be found in Ref. [8] and the parameters of bottomonia are given in (6).

meson	a	b	c	d	α_s
$c\bar{c}$	1.1715	1.2250	0.8087	0.5291	0.36
$b\bar{b}$	1.2165	1.2988	0.8686	0.5886	0.284
$b\bar{c}$ (or $\bar{b}c$)	1.1940	1.2619	0.8387	0.5589	0.322

Since the values of $a\alpha_s$ and $c\alpha_s$ are more useful for the calculation as discussed before, we re-define:

$$A = a\alpha_s \quad \text{and} \quad C = c\alpha_s. \tag{18}$$

Thus the parameters for $b\bar{c}(\bar{b}c)$ mesons are:

$$\begin{cases} A_{bc} = (A_b + A_c)/2; \quad b_{bc} = (b_b + b_c)/2 \\ C_{bc} = (C_b + C_c)/2; \quad d_{bc} = (d_b + d_c)/2 \end{cases}. \tag{19}$$

The difference of the quark masses ($m_c = 1.8$ GeV and $m_b = 4.8$ GeV) makes the Hamiltonian (1) possess a more complicated form [9]:

$$H = H_0 + H_1 + \cdots, \tag{20a}$$

$$H_0 = \frac{p^2}{2\mu} + m_b + m_c + V(r) + S(r), \tag{20b}$$

$$H_1 = H_{sd} + H_{si}, \tag{20c}$$

$$\begin{aligned} H_{sd} &= H_{ls} + H_{ss} + H_t \\ &= \frac{1}{2r}(V'(r) - S'(r))\left(\frac{L\cdot S_b}{m_b^2} + \frac{L\cdot S_c}{m_c^2}\right) \\ &\quad + \frac{V'(r)}{m_b m_c} L\cdot S + \frac{2}{3m_b m_c}\nabla^2 V(r) S_b \cdot S_c \\ &\quad + \frac{1}{m_b m_c}\left(\frac{V'(r)}{r} - V''(r)\right) \\ &\quad \times \left(\frac{(S_b\cdot r)(S_c\cdot r)}{r^2} - \frac{1}{3}S_b\cdot S_c\right), \end{aligned} \tag{21}$$

$$\begin{aligned} H_{si} &= \frac{1}{8}\left(\frac{1}{m_b^2} + \frac{1}{m_c^2} - \frac{2}{m_b m_c}\right)\nabla^2 V(r) \\ &\quad + \frac{1}{4m_b m_c}\left\{\frac{2}{r}V'(r)\cdot L^2 + [p^2, V(r) - rV'(r)]\right. \\ &\quad + 2(V(r) - rV'(r))p^2 \\ &\quad \left. + \frac{1}{2}\left(\frac{8}{r}V'(r) + V''(r) - rV'''(r)\right)\right\}. \end{aligned} \tag{22}$$

So the Schrödinger equation we need is:

$$H\Psi(r) = (H_0 + H_1)\Psi(r) = (E + m_b + m_c)\Psi(r), \tag{23}$$

where,

$$\mu = \frac{m_b m_c}{m_b + m_c}. \tag{24}$$

With this equation and the concerned parameters, we can predict the spectra of the members of the whole $b\bar{c}(\bar{b}c)$ family shown in Table 5.

Table 5. The prediction of the spectra of the B_c meson, where A is with the parameter in Table 4, and B is considering the effect of the Lamb shift and the parameters are taken as (19).

quantity	A	B	EFG [32, 33]	KWLC [34]	quantity	A	B	EFG [32, 33]	KWLC [34]
$1^3S_1 - 1^1S_0$	0.0526	0.0448	0.0620	0.0548	$1^3P_1 - 1^3P_0$	0.0495	0.0411		
$2^1S_0 - 1^1S_0$	0.5923	0.5843	0.5650	0.5863	$1^3P_2 - 1^1P_1$	0.0290	0.0320	0.0280	
$2^3S_1 - 1^3S_1$	0.5723	0.5744	0.5430	0.5795	$1^3D_1 - 2^3S_1$	0.1341	0.1509	0.1910	
$3^3S_1 - 2^3S_1$	0.4021	0.4067	0.3540	0.3652	$1^3D_2 - 1^3D_1$	0.0176	0.0253	0.0050	
$1^3P_0 - 1^3S_1$	0.3709	0.3885	0.3670		$1^3D_3 - 1^3D_2$	0.0170	0.0261	0.0040	
$1^1P_1 - 1^3P_0$	0.0492	0.0392	0.0350						

6 Conclusion and discussion

In this work, we study the role of scalar potential to the spectra of charmonia, bottomonia and the $b\bar{c}(\bar{b}c)$ family. Our strategy is that the scalar and vector potentials have different fractions which manifest in their coefficients (In the text, they are a, b, c and d for the Coulomb and confinement pieces respectively). By fitting some members of charmonia and bottomonia which are more accurately measured, we fix them. Except for B_c, the ground state of the $b\bar{c}(\bar{b}c)$ family, other states have not been well measured yet, so we interpolate the parameters for charmonia and bottomonia to determine the ones concerned for the $b\bar{c}(\bar{b}c)$ mesons. With those parameters, we further predict the mass spectra of the rest resonances of charmonia, bottomonia and the whole $b\bar{c}(\bar{b}c)$ family. It is shown that unlike the QED case where the fraction of the scalar potential is very small and negligible, for the quarkonia where QCD dominates, the fraction of scalar potential is of the same order of magnitude as the vector potential. This is consistent with the conclusion of Ref. [35] and is not surprising. As we indicated that for the vector-like coupling theories QED and QCD, the scalar potential can only appear at loop level or is induced by non-perturbative effects (QCD only). Thus it should be loop-suppressed. However, for QCD, the coupling is sizable and the higher order contributions and the non-perturbative effects somehow are significant, so one can expect the fraction of the scalar potential is large.

Moreover, the Lamb shift is induced by the vacuum fluctuation and only appears at loop level. Indeed its leading contribution is at $O(\alpha_s^2)$. Therefore for the QED case, it is hard to observe the Lamb shift (Observation of the Lamb shift is a great success for theory and experiment indeed), however, for QCD the effects are not ignorable. It is shown [5, 6] that the NLO QCD effects may exceed the LO contributions in some processes. By taking into account the Lamb shift, we re-fit the model parameters and find they are obviously distinct from those without considering the Lamb shift.

The results help us to better understand QCD, higher order effects and especially non-perturbative effects. Even though it is only half-quantitative, it is an insight into the whole picture.

In this work, we adopt the renormalization scheme as $\mu = 2/na_B$ [13], which determines the effective coupling α_s. It is worth emphasizing that α_s depends on the principal quantum number n and this is different from that usually used in the literature. Except for the ground states of charmonia and bottomonia, the values of α_s are quite close to those appearing in the literature.

The predictions for the $b\bar{c}(\bar{b}c)$ family will be tested at LHCb experiments where a great number of the excited states of $b\bar{c}(\bar{b}c)$ will be produced. By comparing the data, we will learn more about QCD and structures of the "final" meson family.

Actually, in this work, we only consider the Cornell potential which is supported by the area theorem and commonly adopted in phenomenological studies of the spectra and wavefunctions of heavy mesons. Indeed, there are some other proposals. For example, the authors of Ref. [36] use the harmonic oscillator model to deal with confinement and further consider the effects of open charm loop for higher excited charmonia states which may induce energy shifts and change decay widths. Moreover, a phenomenological form of the spin-spin interaction [37] which may also result in an energy level shift, is introduced. In this work, we restrict ourselves to quark level QCD motivated potential whose form is given in Refs. [9, 10], but we may further our studies on the coupled-channel scenario in our coming work.

The contribution of the scalar potential to the hadron spectra was noticed by some authors [38] a long time ago, and its importance was confirmed. In this work, we re-emphasize its role and discuss the origin compared with the QED case. In terms of the newly achieved data on charmonia and bottomonia, we analyze the hadron spectra and gain all the concerned parameters. We also investigate the significance of the Lamb shift phenomenologically. Then we go on discussing the spectra of the $b\bar{c}(\bar{b}c)$ family within the same framework, the results will be tested in future experiments.

Appendix A

Check the legitimacy of the approximation $p^4 \sim [2\mu(E_0 - V(r))]^2$

We investigate and elucidate the legitimacy of the approximation adopted in the text:

$$p^4 \sim \left[2\mu(E_0 - V(r))\right]^2$$

through a few examples.

In fact, such problems have been thoroughly discussed in the literature and even written about in textbooks, for example in Ref. [39] and the relativistic corrections to the Cornell potential can be found in Ref. [40]. Here we re-do the numerical computation to convince our readers and ourselves of the legitimacy of the approximation adopted in the text because it is very important in obtaining the spectra.

The 0-th order Schrördinger equation is:

$$\left[\frac{p^2}{2\mu} + V(r)\right]\Psi = E_0\Psi. \tag{A1}$$

With the relativistic correction, it will be:

$$\left[\frac{p^2}{2\mu} + V(r) - \frac{p^4}{4m^3}\right]\Psi = E_1\Psi. \tag{A2}$$

Note: here we ignore other irrelevant correction terms such as the L-S coupling, etc. because we are only concerned with the p^4 term and the approximation.

First, let us use the Coulomb potential as an example because there exists an analytical solution.

For the Coulomb potential:

$$V(r) = -\frac{a}{r}. \tag{A3}$$

We have the exact solution (the eigen-energy and the wave function):

$$E_0^n = -\frac{a^2}{4n^2}, \tag{A4a}$$

$$R_{10}(r) = 2K^{\frac{3}{2}}\mathrm{e}^{-Kr}, \tag{A4b}$$

$$R_{20}(r) = \left(\frac{1}{2}K\right)^{\frac{3}{2}}(2 - Kr)\,\mathrm{e}^{-\frac{1}{2}Kr}, \tag{A4c}$$

$$R_{30}(r) = \left(\frac{1}{3}K\right)^{\frac{3}{2}}\left[2 - \frac{4}{3}K + \frac{4}{27}K^2\right]\mathrm{e}^{-\frac{1}{3}Kr}, \tag{A4d}$$

where,

$$\mu = \frac{m^2}{2m} = \frac{m}{2}; \qquad K = \frac{1}{2}ma.$$

If $m = 1.84$ GeV, and $a = 0.5$ (these numbers are just taken for illustration, but not for real physics), then:

$$\begin{cases} E_0^{n=1} = -0.115, \\ E_0^{n=2} = -0.02875, \\ E_0^{n=3} = -0.012778, \end{cases} \tag{A5}$$

and in the perturbative method, the relativistic correction is:

$$\Delta E^n = \int \mathrm{d}r\; r^2 \frac{1}{4m^3}\left[\boldsymbol{p}^2 R_{n0}(r)\right]^2,$$

$$\Rightarrow \begin{cases} \Delta E^{n=1} = 0.008984; \\ \Delta E^{n=2} = 0.001460; \\ \Delta E^{n=3} = 0.000558. \end{cases} \tag{A6}$$

On the other hand, we use the approximation: $p^4 \sim \left[2\mu(E_0 - V(r))\right]^2$ in Eq. (A2)[1)], and then find the numerical solution of Eq. (A2):

$$\begin{cases} E_1^{n=1} = -0.1223; \\ E_1^{n=2} = -0.0300; \\ E_1^{n=3} = -0.0130. \end{cases} \tag{A7}$$

If we define: $\Delta E_1 = E_0^n - E_1^n$, then we have:

$$\begin{cases} \Delta E_1^{n=1} = 0.007265; \\ \Delta E_1^{n=2} = 0.001249; \\ \Delta E_1^{n=3} = 0.0002288. \end{cases} \tag{A8}$$

From Eqs. (A6) and (A8), we can find that the error is near 0.001 GeV. The relative error is:

$$x^n = \frac{(E_0^n + \Delta E^n) - E_1^n}{(E_0^n + \Delta E^n) + E_1^n},$$

$$\Rightarrow \begin{cases} x^{n=1} = 0.68\%; \\ x^{n=2} = 0.35\%; \\ x^{n=3} = 1.28\%. \end{cases} \tag{A9}$$

With the Coulomb potential the Schrödinger equation possesses an analytical solution, so it is easy to see the error. However, for the Cornell potential, there is no analytical solution available, so we need to use the numerical solution for our analysis.

The Cornell potential is:

$$V(r) = -\frac{a}{r} + br, \tag{A10}$$

where, we set $a = 0.5$, $b = 0.2$ and consider the second radially excited state with $n = 2$ as an example. The numerical solution of Eq. (A1) is:

$$E_0^{n=2} = 0.856872, \tag{A11}$$

and the numerical solution of Eq. (A2) is:

$$E_1^{n=2} = 0.918242. \tag{A12}$$

So we have:

$$\Delta E'^{n=2} = E_1^{n=2} - E_0^{n=2} = 0.06137. \tag{A13}$$

1) here, we may use E_0 as well, but for a clear comparison we use E_1 instead. The error is not great.

In the numerical solution of Eq. (A1) we have the wave function $R_{nl}(r)$, and with the perturbative method, the contribution of the relativistic correction is:

$$\Delta E^{n=2} = \int \frac{1}{4m^3}\left[\boldsymbol{p}^2 R_{20}(r)\right]^2 r^2 \mathrm{d}r = 0.0669. \quad \text{(A14)}$$

Finally, from Eqs. (A13) and (A14), we have the relative error:

$$x^{n=2} = \frac{\left(E_0^{n=2}+\Delta E^{n=2}\right)-E_1^{n=2}}{\left(E_0^{n=2}+\Delta E^{n=2}\right)-E_1^{n=2}} = 0.30\%. \quad \text{(A15)}$$

Even though the relativistic error seems large, in fact the error is only of the order of a few MeV. The QCD Lamb shift generally results in several ten MeV, thus the error brought up by the approximation does not seem too serious.

Here one important point should be clarified. By directly calculating Eq. (A14), one would have an unrealistically large result. The reason is obvious. Unlike the analytical solution for the Coulomb potential, the behavior of the numerical solution near the zero point ($r \to 0$) is not appropriate (namely it does not possess an exponential factor to guarantee the convergence of the solutions). In other words, as $r \to 0$ corresponding $p \to \infty$, the contribution of the power term p^m ($m > 2$) would become larger and larger for higher m. Indeed all higher power terms should exist in relativistic corrections. Integration over the wavefunction would blow up. Thus the whole picture is not acceptable. To remedy it, there are two ways. One is to introduce an exponential convergence factor and another is to restrict the integration region, i.e. one does not integrate from $r = 0$, but sets the lower bound to be a small number δ. Definitely, one should find a small value of δ and when its value changes slightly, the result does not vary much. Thus we would convince ourselves that this integration is reliable. The second way is much simpler than the first one, and we adopt it for the above calculation. We carefully discussed such virtual singularity in our earlier paper [19].

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