Spectroscopy of heavy mesons expanded in $1/m_Q$

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Starting from the semirelativistic Hamiltonian for a $Q\overline{q}$ system with Coulomb and linear confining scalar potentials, and operating just once with the naive Foldy-Wouthuysen-Tani transformation on the heavy quark, we have calculated the heavy meson mass spectra of D and B together with higher spin states. Based on the formulation recently proposed, their masses and wave functions are expanded up to second order in $1/m_Q$ with a heavy quark mass m_Q and the lowest-order equation is examined carefully to obtain a complete set of eigenfunctions for the Schrödinger equation. Heavy quark effective theory parameters $\overline{\Lambda}$, λ_1, and λ_2 are also determined at first and second order in $1/m_Q$. [S0556-2821(97)06521-1]

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I. INTRODUCTION

Hadrons are composed of quarks and antiquarks and are considered to be governed by quantum chromodynamics (QCD), at least in principle. Since QCD describes a strong coupling interaction, a perturbative calculation of physical quantities of hadrons is not so reliable other than in the deep inelastic region where the coupling constant becomes weak due to asymptotic freedom and hence other methods such as lattice gauge theory have been developed to take into account nonperturbative effects. However, the situation dramatically changes when it is discovered that the system of heavy hadrons, composed of one heavy quark Q and light quarks q or antiquarks $\overline{q}$, can be systematically expanded in $1/m_Q$ with a heavy quark mass m_Q. The numerator of this expansion in $1/m_Q$ could be either $\Lambda_{\rm QCD}$ or m_q.

This theory, heavy quark effective theory (HQET) [1] is applied to many aspects of high-energy theories and many kinds of physical quantities of QCD which can be perturbatively calculated in $1/m_Q$. Especially those regarding B meson physics, e.g., the lowest order form factor (which is now called Isgur-Wise function) of the semileptonic weak decay process $B\to D\ell\nu$ and the Kobayashi-Maskawa matrix element V_{cb}, have been calculated by many people [2]. However, since applications of HQET to higher-order perturbative calculations are very restricted, only forms of higher-order operators are obtained. Their Wilson coefficients are calculable, but some of the matrix elements of those operators are obtained so that the whole quantity be somehow fitted with the experimental data [3]. This is because most of the calculations based on HQET do not introduce realistic heavy meson wave functions and hence there is no way to determine those quantities completely within the model.

In previous papers [4,5], using the Foldy-Wouthuysen-Tani transformation [6] we have developed a formulation so that the Schrödinger equation for a $Q\overline{q}$ bound state can be expanded in terms of $1/m_Q$; i.e., the resulting eigenvalues as well as wave functions are obtained order by order in $1/m_Q$. In this paper, as one of the applications of our formulation we will calculate the heavy meson spectra of D and B, and their higher spin states. In order to do so, we would like to start from introducing phenomenological dynamics, i.e., assuming Coulomb-like vector and confining scalar potentials to $Q\overline{q}$ bound states (heavy mesons), expand a Hamiltonian in $1/m_Q$ then perturbatively solve the Schrödinger equation in $1/m_Q$. Angular part of the lowest-order wave function is exactly solved. After extracting asymptotic forms of the lowest-order wave function at both $r\to 0$ and $r\to\infty$ and adopting the variational method, we numerically obtain the radial part of the trial polynomial wave function which is expanded in powers of radial variable r. Then fitting the smallest eigenvalues of a Hamiltonian with masses of D and D^* mesons, a strong coupling α_s, and other parameters included in scalar and vector potentials are determined uniquely. Using parameters obtained this way, other mass levels are calculated and compared with the experimental data for D/B mesons up to the second order of perturbation. The lowest degenerate eigenvalues of the Schrödinger equation gives the so-called $\overline{\Lambda}$ parameters for u, d, and s light quarks, which is defined by

$$\overline{\Lambda}=\lim_{m_Q\to\infty}(E_H-m_Q),$$

where E_H is a calculated heavy meson mass and m_Q a heavy quark mass [3]. Meson wave functions obtained thereby and expanded in $1/m_Q$ may be used to calculate ordinary form factors as well as Isgur-Wise functions and its corrections in $1/m_Q$ for semileptonic weak decay processes.

All the above calculations are calculated up to $1/m_Q^2$ and analyzed order by order in $1/m_Q$ to determine parameters as well as to compare with results of heavy quark effective theory, e.g., the parameters, λ_1, λ_2, and $\overline{\Lambda}$ in Sec. IV. The final goal of this approach is to obtain higher-order correc-

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tions to Isgur-Wise functions, decay constants of heavy mesons, and the Kobayashi-Maskawa matrix element, V_{cb}, by using wave functions of heavy mesons obtained so that heavy meson spectrum is fitted with the experimental data.

Below in Secs. II and III we will first give formulation of this study and next in Secs. IV and V give quantitative and qualitative discussions on the obtained results.

II. HAMILTONIAN

The Hamiltonian density for our problem is given by

$$\mathcal{H}_0=\int dx^3\ [q^{\dagger\, c}(x)\ (\vec{\alpha}_q\cdot\vec{p}_q+\beta_q m_q)\ q^c(x) + Q^{\dagger}(x)(\vec{\alpha}_Q\cdot\vec{p}_Q+\beta_Q m_Q)Q(x)\ ], \tag{1}$$

$$\mathcal{H}_{\rm int}=\int\int dx^3 dx'^3\overline{q^c(x)}O_i q^c(x) \times V_i(x-x')\overline{Q(x')}O_i Q(x'), \tag{2}$$

where we consider only a scalar confining potential, $O_s=1, V_s=S(r)$, and a vector potential, $O_v=\gamma_\mu, V_v=V(r)$, with a relative radial variable r, which we think is the best choice to describe phenomenologically the meson mass levels [7,8]. The state of $Q\overline{q}$ is defined by

$$|\psi\rangle=\int d^3x\int d^3y\,\psi_{\alpha\beta}(x-y)q^{c\,\dagger}_{\alpha}(x)Q^{\dagger}_{\beta}(y)|0\rangle, \tag{3}$$

where $q^c(x)$ is a charge conjugate field of a light quark q and the conjugate state of $Q\overline{q}$ by $\langle\psi|=|\psi\rangle^{\dagger}$ with $\langle 0|\equiv|0\rangle^{\dagger}$. From these definitions, we obtain the Fermi-Yang equation [9] or the Schrödinger equation as

$$H\psi=(m_Q+\widetilde{E})\psi, \tag{4}$$

where the bound state mass, E, is split into two parts, m_Q and $\widetilde{E}$ $(=E-m_Q)$, so that it expresses the fact that the heavy quark mass is dominant in the bound state, $Q\overline{q}$, and ψ is nothing, but the wave function which appears in the right-hand side (RHS) of Eq. (3).

Operating with the FWT transformation and a charge conjugation operator, which are defined in Appendix A, only on the heavy quark sector in this equation at the center of the mass system of a bound state, one can modify the Schrödinger equation given by Eq. (4) as

$$(H_{\rm FWT}-m_Q)\otimes\psi_{\rm FWT}=\widetilde{E}\psi_{\rm FWT}, \tag{5}$$

where a notation $\otimes$ is introduced to denote that gamma matrices of a light anti-quark is multiplied from left while those of a heavy quark from right or, more explicitly,

$$\mathcal{O}_q\mathcal{O}_Q\otimes\psi_{\rm FWT}=(\mathcal{O}_q)_{\alpha\beta}(\psi_{\rm FWT})_{\beta\gamma}(\mathcal{O}_Q)_{\gamma\delta}, \tag{6}$$

where $\mathcal{O}_q$ and $\mathcal{O}_Q$ represent gamma matrices related to light anti-quark and heavy quark, respectively. The problem of this paper is to solve this equation, Eq. (5), in powers of $1/m_Q$. As described first in this section, interaction terms are given by a confining scalar potential and a Coulomb vector potential with transverse interaction [10] and a total Hamiltonian is given by

$$H=(\vec{\alpha}_q\cdot\vec{p}_q+\beta_q m_q)+(\vec{\alpha}_Q\cdot\vec{p}_Q+\beta_Q m_Q)+\beta_q\beta_Q\ S +\{1-\tfrac{1}{2}[\vec{\alpha}_q\cdot\vec{\alpha}_Q+(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})\ ]\}V, \tag{7}$$

where scalar and vector potentials are given by

$$S(r)=\frac{r}{a^2}+b,\quad V(r)=-\frac{4}{3}\frac{\alpha_s}{r},\quad\text{and}\quad \vec{n}=\frac{\vec{r}}{r}, \tag{8}$$

and the vector potential is averaged over longitudinal as well as transverse as given in the last term of Eq. (7). The transformed Hamiltonian is expanded in $1/m_Q$ as

$$H_{\rm FWT}-m_Q=H_{-1}+H_0+H_1+H_2+\cdots, \tag{9}$$

where

$$H_{-1}=-(1+\beta_Q)m_Q, \tag{10a}$$

$$H_0=\vec{\alpha}_q\cdot\vec{p}+\beta_q m_q-\beta_q\beta_Q\ S+\{1+\tfrac{1}{2}[\ \vec{\alpha}_q\cdot\vec{\alpha}_Q +(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})\ ]\}V, \tag{10b}$$

$$H_1=-\frac{1}{2\,m_Q}\beta_Q\ \vec{p}^{\,2}+\frac{1}{m_Q}\beta_q\ \vec{\alpha}_Q\cdot\left(\vec{p}+\frac{1}{2}\vec{q}\right)\ S+\frac{1}{2m_Q}\vec{\gamma}_Q\cdot\vec{q}V -\frac{1}{2m_Q}\left[\beta_Q\left(\vec{p}+\frac{1}{2}\vec{q}\right)+i\ \vec{q} \times\beta_Q\ \vec{\Sigma}_Q\right]\cdot[\ \vec{\alpha}_q+(\vec{\alpha}_q\cdot\vec{n})\vec{n}\ ]V, \tag{10c}$$

$$H_2=\frac{1}{2m_Q^2}\ \beta_q\beta_Q\ \left(\vec{p}+\frac{1}{2}\vec{q}\right)^2 S-\frac{i}{4m_Q^2}\vec{q}\times\vec{p}\cdot\beta_q\beta_Q\ \vec{\Sigma}_Q\ S -\frac{1}{8m_Q^2}\vec{q}^{\,2}V-\frac{i}{4m_Q^2}\vec{q}\times\vec{p}\cdot\vec{\Sigma}_Q\ V -\frac{1}{8m_Q^2}\{(\vec{p}+\vec{q})\ (\vec{\alpha}_Q\cdot\vec{p}) +\vec{p}[\vec{\alpha}_Q\cdot(\vec{p}+\vec{q})]+i\vec{q}\times\vec{p}\ \ \gamma_Q^5\}\cdot[\ \vec{\alpha}_q+(\vec{\alpha}_q\cdot\vec{n})\vec{n}\ ]\ V, \tag{10d}$$

$$\vdots$$

Here H_i stands for the ith order expanded Hamiltonian, the Dirac gamma matrices, β, $\vec{\alpha}$, and $\vec{\Sigma}$ are defined as

$$\beta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad \vec{\alpha}=\begin{pmatrix}0 & \vec{\sigma}\\ \vec{\sigma} & 0\end{pmatrix},\quad \vec{\Sigma}=\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}, \tag{11}$$

and since a bound state is at rest,

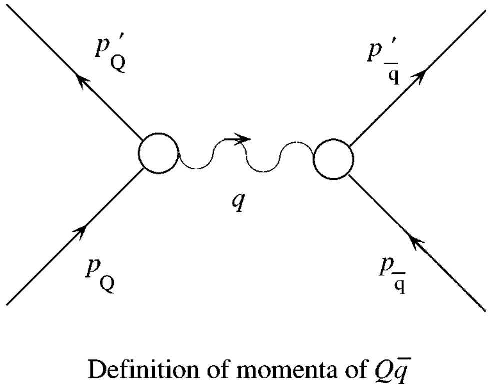

FIG. 1. Each momentum is defined.

$$\vec p = \vec p_q = -\vec p_Q, \quad \vec p\,' = \vec p_q\,' = -\vec p_Q\,', \quad \vec q = \vec p\,' - \vec p, \quad (12)$$

are defined, where primed quantities are final momenta and the relation of these momenta with particles is depicted in Fig. 1.

Details of derivation of equations in this section are given in Appendix A.

III. PERTURBATION

Using the Hamiltonian obtained in the last section, we give in this section the Schrödinger equation order by order in $1/m_Q$. Details of the derivation in this section are given in Appendix B. First we introduce the projection operators:

$$\Lambda_{\mp} = \frac{1 \mp \beta_Q}{2}, \quad (13)$$

which correspond to positive-/negative-energy projection operators for a heavy quark sector at the rest frame of a bound state. The notation might be confusing since these expressions are opposite to the ordinary definition. As described just before Eq. (5) or at the end of Appendix A, heavy quarks in the Schrödinger equation are transformed by the charge conjugation operator, U_c, and the projection operators are given by Eq. (A5) or in the present notation using $\otimes$ by Eq. (13). These correspond to $(1 \pm \not v)/2$ in a moving frame of a bound state with v^μ the four-velocity of a bound state. Then we expand the mass and wave function of a bound state in $1/m_Q$ as

$$\widetilde E = E - m_Q = E_0^\ell + E_1^\ell + E_2^\ell + \cdots, \quad (14)$$

$$\psi_{\rm FWT} = \psi_0^\ell + \psi_1^\ell + \psi_2^\ell + \cdots, \quad (15)$$

where ℓ stands for a set of quantum numbers that distinguish independent eigenfunctions of the lowest-order Schrödinger equation, and a subscript i of E_i^ℓ and ψ_i^ℓ stands for the order of $1/m_Q$.

A. −1st order

The −1st-order Schrödinger equation in $1/m_Q$ gives a 4×4 matrix wave function as

$$\psi_0^\ell = \Lambda_- \otimes \psi_0^\ell = \psi_0^\ell\ \Lambda_-, \quad (16)$$

whose explicit form is solved in Appendix C and is given by

$$\psi_0^\ell = \Psi_\ell^+ = (0 \quad \Psi_{j\ m}^k(\vec r)). \quad (17)$$

The notation might be confusing; however, one may understand Eq. (16) by noting

$$U_c \Lambda_+ U_c^{-1} \otimes \psi_0^\ell = \Lambda_- \otimes \psi_0^\ell = \psi_0^\ell \Lambda_-.$$

Here ℓ stands for a set of quantum numbers, j, m, and k and a 4×2 matrix wave function, $\Psi_{j\ m}^k(\vec r)$, is given by

$$\Psi_{j\ m}^k(\vec r) = \frac{1}{r}\begin{pmatrix} u_k(r) \\ -i\ v_k(r)(\vec\sigma\cdot\vec n)\end{pmatrix} y_{j\ m}^k(\Omega), \quad (18)$$

where j is a total angular momentum of a meson, m is its z component, k is a quantum number which takes only values, $k = \pm j,\ \pm(j+1)$ and $\neq 0$, $u_k(r)$ and $v_k(r)$ are scalar polynomials of a radial variable r, and are tacitly assumed to be multiplied by a 2×2 unit matrix. $y_{j\ m}^k(\Omega)$ are functions of angles and 2×2 matrix bi-spinors of a total angular momentum, $\vec j = \vec\ell + \vec s_q + \vec s_Q$ with a definition of an orbital angular momentum $\vec\ell = -i\vec r \times \nabla$, and $\vec s_q$ and $\vec s_Q$ being spin operators of light anti-quark and heavy quark, respectively. Note again that the positive projection operator of a heavy quark is given by Λ_- instead of Λ_+ as described early in this section and should be multiplied from right as shown in Eq. (16). The corresponding operator for the quantum number k is given by [4]

$$-\beta_q(\vec\Sigma_q\cdot\vec\ell + 1), \quad (19)$$

which satisfies

$$-\beta_q(\vec\Sigma_q\cdot\vec\ell + 1)(0 \quad \Psi_{j\ m}^k(\vec r)) = k(0 \quad \Psi_{j\ m}^k(\vec r)), \quad (20)$$

i.e.,

$$[-\beta_q(\vec\Sigma_q\cdot\vec\ell + 1),\ H_0^{--}] = 0, \quad (21)$$

with H_0^{--} being given in Appendix D, the lowest-order nontrivial Hamiltonian,

$$H_0^{--} \otimes \psi_0^\ell = E_0^k \psi_0^\ell.$$

The operator given by Eq. (19) has a form of the spin-orbit coupling of light anti-quark and so is an intrinsic property of the light degree of freedom. Therefore pairs of states with the same value of k are in the near-degeneracy in mass, e.g., the two states of $J^P = 0^-, 1^-$ with $k = -1$, whose details are described at the end of Appendix C.

Note that since charge conjugation operates on the heavy quark sector, the Λ_- projection operator appears in Eq. (16), i.e., positive components of Q corresponds to negative components of $U_c Q$.

B. Zeroth order

The zeroth order equations are given by

$$[\vec{\alpha}_q\cdot\vec{p}+\beta_q(m_q+S)+V\,]\otimes\psi_0^{\ell}=E_0^{\ell}\;\psi_0^{\ell}, \qquad (22)$$

$$-2m_Q\Lambda_+\otimes\psi_1^{\ell}+\tfrac{1}{2}\,\Lambda_-[\vec{\alpha}_q\cdot\vec{\alpha}_Q+(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})\;]V\otimes\psi_0^{\ell} =0. \qquad (23)$$

Equation (22) gives the lowest nontrivial Schrödinger equation with a solution given by Eq. (17) and $\vec{n}=\vec{r}/r$. A detailed analysis of this equation is given in Appendix C. Λ_+ components of wave functions can be expanded in terms of the eigenfunctions:

$$\Psi_{\ell}^{-}=(\Psi_{j\;m}^{k}(\vec{r})\;\;0). \qquad (24)$$

Expanding $\Lambda_+\otimes\psi_1^{\ell}$ in terms of this set of eigenfunctions, one can obtain the solution for Eq. (23) as

$$\Lambda_+\otimes\psi_1^{\ell}=\sum_{\ell'}\;c_{1-}^{\ell\,\ell'}\Psi_{\ell'}^{-}, \qquad (25)$$

with the coefficients

$$c_{1-}^{\ell\,\ell'}=\frac{1}{4m_Q}\langle\Psi_{\ell'}^{-}|[\vec{\alpha}_q\cdot\vec{\alpha}_Q+(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})\;]V|\Psi_{\ell}^{+}\rangle. \qquad (26)$$

Here the inner product is defined to be

$$\langle\Psi_{\ell}^{\alpha}|O|\Psi_{\ell'}^{\beta}\rangle=\int d^3r\;\mathrm{tr}[\Psi_{\ell}^{\alpha\dagger}(O\otimes\Psi_{\ell'}^{\beta})], \qquad (27)$$

where the notation $\otimes$ is defined by Eq. (6) and the zeroth order wave functions are normalized to be 1:

$$\langle\Psi_{\ell}^{\alpha}|\Psi_{\ell'}^{\beta}\rangle=\delta_{\ell\,\ell'}\delta^{\alpha\,\beta}\quad\text{for }\alpha,\;\beta=+\;-. \qquad (28)$$

C. 1st order

The 1st-order equation is given by

$$-2m_Q\Lambda_+\otimes\psi_2^{\ell}+H_0\otimes\psi_1^{\ell}+H_1\otimes\psi_0^{\ell}=E_0^{\ell}\psi_1^{\ell}+E_1^{\ell}\psi_0^{\ell}. \qquad (29)$$

Multiplying projection operators $\Lambda_\pm$ from right with the above equation, and expanding ψ_1^{ℓ} in terms of $\Psi_{\ell}^{\pm}$ as

$$\psi_1^{\ell}=\sum_{\ell}\;(c_{1+}^{\ell\,\ell'}\Psi_{\ell'}^{+}+c_{1-}^{\ell\,\ell'}\Psi_{\ell'}^{-}), \qquad (30)$$

one obtains

$$E_1^{\ell}=\sum_{\ell'}\;c_{1-}^{\ell\,\ell'}\langle\Psi_{\ell}^{+}|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^{-}\rangle +\langle\Psi_{\ell}^{+}|\Lambda_-H_1\Lambda_-|\Psi_{\ell}^{+}\rangle, \qquad (31)$$

which gives the first-order perturbation correction to the mass when one calculates matrix elements of the RHS among eigenfunctions and

$$c_{1+}^{\ell\,k}=\frac{1}{E_0^{\ell}-E_0^{k}}\left[\sum_{\ell'}\;c_{1-}^{\ell\,\ell'}\langle\Psi_k^{+}|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^{-}\rangle +\langle\Psi_k^{+}|\Lambda_-H_1\Lambda_-|\Psi_{\ell}^{+}\rangle\right],\quad\text{for }k\neq\ell, \qquad (32)$$

$$c_{1+}^{k\,k}=0. \qquad (33)$$

This completes the solution for ψ_1^{ℓ} since $\Lambda_+\otimes\psi_1^{\ell}$, or $c_{1-}^{\ell\,\ell'}$, is obtained in the last subsection. Here we have used the normalization for the total wave function, ψ^{ℓ}, as

$$\langle\psi^{\ell}|\psi^{\ell'}\rangle=\delta_{\ell\,\ell'}, \qquad (34)$$

where we have neglected color indices in this paper and hence a color factor, $N_c=3$, in the above equation since it does not change the essential arguments. This definition of Eq. (34) is admitted because here we are not calculating the absolute value of the form factors. The appropriate normalization (normally given by $2E$ with a bound state mass E) will be adopted in future papers in which we will calculate some form factors. This way of obtaining the expressions for E_1^{ℓ} and $c_{1\pm}^{\ell\,k}$ by manipulating Eq. (29) is unique and we will use this method below to obtain similar expressions appearing in Sec. III D. Actually this method has been already used to obtain Eqs. (22) and (23) and to solve Eq. (23) obtaining the coefficients $c_{1-}^{\ell\,\ell'}$ by Eq. (26).

One obtains $\Lambda_+\otimes\psi_2^{\ell}$ as in the former subsection,

$$\Lambda_+\otimes\psi_2^{\ell}=\sum_{\ell'}\;c_{2-}^{\ell\,\ell'}\Psi_{\ell'}^{-}, \qquad (35)$$

with the coefficients

$$c_{2-}^{\ell\,\ell'}=\frac{1}{2m_Q}\langle\Psi_{\ell'}^{-}|[(H_0-E_0^{\ell})\Lambda_+\otimes\psi_1^{\ell}+H_1\Lambda_+\otimes\psi_0^{\ell}]\rangle. \qquad (36)$$

D. 2nd order

The 2nd-order equation is given by

$$-2m_Q\Lambda_+\otimes\psi_3^{\ell}+H_0\otimes\psi_2^{\ell}+H_1\otimes\psi_1^{\ell}+H_2\otimes\psi_0^{\ell} =E_0^{\ell}\psi_2^{\ell}+E_1^{\ell}\psi_1^{\ell}+E_2^{\ell}\psi_0^{\ell}. \qquad (37)$$

As in the above case (1st order), we obtain

$$E_2^{\ell}=\sum_{\ell'}\;c_{2-}^{\ell\,\ell'}\langle\Psi_{\ell}^{+}|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^{-}\rangle+\langle\Psi_{\ell}^{+}|H_1\Lambda_-\otimes\psi_1^{\ell}\rangle +\langle\Psi_{\ell}^{+}|\Lambda\_H_2\Lambda_-|\Psi_{\ell}^{+}\rangle, \qquad (38)$$

which gives the second-order perturbation corrections to the mass and

TABLE I. Input values to determine parameters (units are in GeV).

$m_q=m_u=m_d$	M_D	M_{D*}	M_{D_s}	$M_{D_s^*}$	M_B	M_{B*}
0.01	1.867	2.008	1.969	2.112	5.279	5.325

$$c_{2+}^{\ell\, k}=\frac{1}{E_0^\ell-E_0^k}\Bigg[\sum_{\ell'} c_{2-}^{\ell\,\ell'}\langle\Psi_k^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_k^+|\Lambda_+H_1\otimes\psi_1^\ell\rangle+\langle\Psi_k^+|\Lambda_-H_2\Lambda_-|\Psi_\ell^+\rangle-E_1^\ell\, c_{1+}^{\ell\, k}\Bigg],\quad \text{for } k\neq\ell, \tag{39}$$

$$c_{2+}^{k\,k}=-\frac{1}{2}\sum_\ell (|c_{1+}^{k\,\ell}|^2+|c_{1-}^{k\,\ell}|^2). \tag{40}$$

This completes the solution for ψ_2^k since $\Lambda_-\psi_2^k$, or $c_{2-}^{\ell\,\ell'}$, is obtained in the last subsection.

Although we do not need in this paper, one obtains $\Lambda_+\otimes\psi_3^\ell$ as

$$\Lambda_+\otimes\psi_3^\ell=\sum_{\ell'} c_{3-}^{\ell\,\ell'}\Psi_{\ell'}^-, \tag{41}$$

with the coefficients

$$c_{3-}^{\ell\,\ell'}=\frac{1}{2m_Q}\langle\Psi_{\ell'}^-|[(H_0-E_0^\ell)\Lambda_+\otimes\psi_2^\ell+(H_1-E_1^\ell)\Lambda_+\otimes\psi_1^\ell+H_2\Lambda_+\otimes\psi_0^\ell]\rangle. \tag{42}$$

IV. NUMERICAL ANALYSIS

In this section, we give numerical analysis of our analytical calculations obtained in the former sections order by order in $1/m_Q$. In order to solve Eq. (22), we have to obtain numerically a radial part of the wave function, $\Psi_\ell^+=(0\ \ \Psi_{j\,m}^k)$, given by

$$\Psi_{j\,m}^k(\vec r)=\frac{1}{r}\begin{pmatrix} u_k(r)\\ -i\ v_k(r)(\vec\sigma\cdot\vec n)\end{pmatrix}y_{j\,m}^k(\Omega), \tag{43}$$

detailed properties of which are described in Appendix C. As described in the same Appendix, the lowest-order, nontrivial Schrödinger equation is reduced into Eq. (C25):

$$\begin{pmatrix} m_q+S+V & -\partial_r+\frac{k}{r}\\ \partial_r+\frac{k}{r} & -m_q-S+V\end{pmatrix}\begin{pmatrix}u_k(r)\\ v_k(r)\end{pmatrix}=E_0^k\begin{pmatrix}u_k(r)\\ v_k(r)\end{pmatrix}. \tag{44}$$

This eigenvalue equation is numerically solved by taking into account the asymptotic behaviors at both $r\to0$ and $r\to\infty$ and the forms of scalar functions, $u_k(r)$ and $v_k(r)$, are given by

$$u_k(r),\ \ v_k(r)\sim w_k(r)\left(\frac{r}{a}\right)^\gamma \exp\left[-(m_q+b)\ r-\frac{1}{2}\left(\frac{r}{a}\right)^2\right], \tag{45}$$

where

$$\gamma=\sqrt{k^2-\left(\frac{4\alpha_s}{3}\right)^2} \tag{46}$$

and $w_k(r)$ is a finite series of a polynomial of r

$$w_k(r)=\sum_{i=0}^{N-1} a_i^k\left(\frac{r}{a}\right)^i, \tag{47}$$

which takes different coefficients for $u_k(r)$ and $v_k(r)$.

(i) We have fixed the value of a light quark mass, m_q, to be 0.01 GeV as listed in Table I since only in the vicinity of this value the D and D^* masses can be fitted with the experimental values. We believe that when the mass, $m_q=m_u=m_d$, is running with momentum, these are close to the current quark mass since the momentum is given by the order of the B meson mass ($\sim$5 GeV) [14] though we have not used the running mass to solve the Schrödinger equation. From Eqs. (44)–(47), we have a $2N$ dimensional eigenvalue matrix. The lowest eigenvalue of the positive energies is assigned to the physical state adopted here, whose wave function has no node. In practice, we have found that the eigenvalue equation with $N=8$ gives the zero node solution for the lowest positive eigenvalue, while other N gives a rather oscillatory solution, i.e., a solution with some nodes for the lowest positive eigenvalue. Therefore we have adopted $N-1=7$ for the highest power of r that gives sixteen solutions to Eq. (44), half of which corresponds to negative energies and another half to positive ones of q^c state. That is, although we have a node quantum number, n, other than j, m, and k, for Eq. (44), we take only the $n=0$ solution for each value of k and j quantum numbers and we do not assign higher node solutions to any physical states in this paper.

In the case of a hydrogen atom, for instance, only the Coulomb potential $V\sim1/r$ survives in the above problem and a radial function, $w_k(r)$, becomes a hypergeometric function

TABLE II. Most optimal values of parameters determined by the least chi square method.

Parameters	α_s	a (GeV^{-1})	b (GeV)	m_c (GeV)	m_s (GeV)	m_b (GeV)
first order	0.3998	2.140	−0.04798	1.457	0.09472	4.870
second order	0.2834	1.974	−0.07031	1.347	0.08988	4.753

TABLE III. D meson mass spectrum (first order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	M_{calc}	M_{obs}
$^1S_0$ (0^-)	1.869	-2.01 ($\times 10^{-2}$)	1.93 ($\times 10^{-2}$)	1.867	1.867
$^3S_1$ (1^-)		7.37	0.101	2.008	2.008
$^3P_0$ (0^+)	2.276	-0.373	1.59	2.304	-
“$^3P_1$” (1^+)		7.50	0.0883	2.449	2.422(?)
“$^1P_1$” (1^+)	2.216	7.51	0.0210	2.383	-
$^3P_2$ (2^+)		9.54	4.72×10^{-7}	2.428	2.459
$^3D_1$ (1^-)	2.440	181	0.0242	6.850	-
“$^3D_2$” (2^-)		177	4.28×10^{-7}	6.747	-

and its finite series of a polynomial gives discrete energy levels. In our case, since the potential includes a scalar term, we cannot analytically solve the above reduced Schrödinger equation, Eq. (44). If we force to make the functions, $u_k(r)$ and $v_k(r)$, finite series and relate the coefficients of those functions via recursive equations, it leads us to inconsistency among coefficients of each term, r^i, of a polynomial. We just assume in this paper that $u_k(r)$ and $v_k(r)$ are trial finite polynomial functions of r.

(ii) To determine the parameters, α_s, a, and b appearing in the potentials given by Eq. (8), and the quark masses, m_c, m_b, and m_s, we have calculated the chi square defined by

$$\chi^2=\sum_{X=D,D^*,D_s,D_s^*,B,B^*}\frac{(M_X-E_X)^2}{\sigma_X^2}, \qquad (48)$$

where M_X and E_X are the observed and calculated masses of a meson X, respectively, and σ_X is the experimental error for each meson mass. As mentioned already $m_q=m_d=m_u$ is fixed to be 10 MeV. Mass, e.g., M_D, is averaged over charges, $M_{D^\pm}$ and M_{D^0}, since we have not taken into account the electromagnetic interaction, the same is true for M_{D^*}, etc. We have determined the values for these six parameters, α_s, a, b, m_c, m_b, and m_s, by setting the value of χ^2 as 10^{-4}. The input values are given in Table I.

(iii) There are two types of solutions to optimal values for these parameters, i.e., one set for $b<0$ which is listed in Table II, and another for $b>0$. However, the solution for $b>0$ gives large difference between calculated values and observed ones for higher order spins and also gives negative values for some spectrum even though the lowest lying states are in good agreement with the observed ones. Hence we disregard this set of parameters.

Tables III–X give calculated values, M_{calc}, together with the zeroth order masses, M_0 that are degenerate with the same value of k, ratios, p_i/M_0 and n_i/M_0, and the observed values, M_{obs}. Here the heavy meson mass, E_H, is expanded in $1/m_Q$ up to the nth order as

$$E_H=M_0+\sum_{i=1}^{n} p_i+\sum_{i=1}^{n} n_i, \qquad (49)$$

with $M_0=m_Q+E_0$ being the degenerate mass, p_i the ith order correction from positive components of a heavy meson wave function, and n_i the ith order correction from negative components. Note also that the exponential factor in the brackets in the first row of each table should be multiplied with a value of each column except for those with the explicit exponential factor.

Strictly speaking each state is classified by two quantum numbers, k and j, and also approximately classified by the upper component of the light anti-quark sector in terms of the usual notation, $^{2S+1}L_J$. Studying the functions $y^k_{j\,m}$ carefully, one finds the upper component of $\Psi^k_{j\,m}(\vec{r})$ corresponds to the following Table XI, respectively. Here J in J^P and $^{2S+1}L_J$ is the same as a total angular momentum, j, in the Table XI. Although the states can be completely classified in terms of two quantum numbers, k and j, we would like ordinarily to classify them in terms of $^{2S+1}L_J$. However, the states classified by $J^P=1^+$ and 2^-, are mixtures of two states in terms of $^{2S+1}L_J$ as given by the Table XI. We would approximately regard the state $(k,\, j)=(1,\, 1)$ with “$^3P_1$,” $(-2,\, 1)$ with “$^1P_1$” and $(2,\, 2)$ with “$^3D_2$,” respectively, whose legitimacy can be supported by calculating the coefficient of each state $^{2S+1}L_J$ included in the mixture state. We denote them with double quotations so that they

TABLE IV. D_s meson mass spectrum (first order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	M_{calc}	M_{obs}
$^1S_0$ (0^-)	1.986	$-2.66(\times 10^{-2})$	$1.67(\times 10^{-2})$	1.966	1.969
$^3S_1$ (1^-)		6.95	0.0851	2.125	2.112(?)
$^3P_0$ (0^+)	2.288	0.769	1.45	2.339	-
“$^3P_1$” (1^+)		8.62	0.0835	2.487	2.535
“$^1P_1$” (1^+)	2.335	6.87	0.0194	2.496	-
$^3P_2$ (2^+)		8.79	8.87×10^{-7}	2.540	2.574(?)
$^3D_1$ (1^-)	2.401	159	0.0282	6.230	-
“$^3D_2$” (2^-)		126	8.63×10^{-7}	5.428	-

TABLE V. B meson mass spectrum (first order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	5.281	$-2.13(\times 10^{-3})$	$2.05(\times 10^{-3})$	5.281	5.279
$^3S_1$ (1^-)		7.80	0.107	5.323	5.325
$^3P_0$ (0^+)	5.689	-0.447	1.90	5.697	-
‘‘$^3P_1$’’ (1^+)		8.98	0.106	5.740	-
‘‘$^1P_1$’’ (1^+)	5.629	8.85	0.0247	5.679	-
$^3P_2$ (2^+)		11.2	5.56×10^{-8}	5.692	-
$^3D_1$ (1^-)	5.853	225	0.0302	7.172	-
‘‘$^3D_2$’’ (2^-)		220	5.34×10^{-8}	7.141	-

remind us an approximate representation of the state in terms of $^{2S+1}L_J$. Using Eq. (C6) in Appendix C, their relations are given by

$$\begin{pmatrix} |``^3P_1"\rangle \\ |``^1P_1"\rangle \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{2} & 1 \\ -1 & \sqrt{2} \end{pmatrix} \begin{pmatrix} |^3P_1\rangle \\ |^1P_1\rangle \end{pmatrix}, \tag{50}$$

$$\begin{pmatrix} |``^3D_2"\rangle \\ |``^1D_2"\rangle \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} \sqrt{3} & \sqrt{2} \\ -\sqrt{2} & \sqrt{3} \end{pmatrix} \begin{pmatrix} |^3D_2\rangle \\ |^1D_2\rangle \end{pmatrix}. \tag{51}$$

(iv) From Tables III–X we see that the perturbative calculation with these parameters might not work well for higher k. Namely masses of 1^- and 2^- for $k=+2$ give some odd values. They become even negative for ‘‘$^3D_2$’’ of D_s and B_s at the second order as shown in Tables VIII and X. Hence we disregard in this paper all calculated masses of $^3D_1(1^-)$ and ‘‘$^3D_2$’’(2^-) states in any order. In order to remedy this problem, we may need to improve the potential form or adopt some other methods [15]. Hence here only the first-order mass spectra are depicted without higher spin states [$^3D_1(1^-)$ and ‘‘$^3D_2$’’(2^-)] in Figs. 2–5.

One may also notice that the s quark mass listed in Table II is relatively small ($\sim$90 MeV) compared with the conventionally used values, $\sim$150 GeV, which is regarded as the current quark mass. It is interesting to note that these values are also obtained as $\overline{m_s}(\mu=2\,\text{GeV})$ in the recent lattice QCD calculations [16].

(v) Two states, pseudoscalar (0^-) and vector (1^-), are degenerate at the zeroth order in $1/m_Q$ since the eigenvalue E_0^k for these states depends on the same quantum number $k=-1$, which are split into two via the heavy quark spin interaction terms, like $-V'(\vec{\alpha}_q\cdot\vec{\Sigma}_Q\times\vec{n})$ in H_1^{--} and all terms in H_1^{-+} given by Eq. (D10). Similar resolution of the degeneracy among the states with the same value of k occurs via the same interaction terms.

(vi) The simple-minded heavy meson mass formula given by

$$m_c\ (E_{D*}-E_D)=m_b\ (E_{B*}-E_B) \tag{52}$$

holds exactly at the first order calculation. This is because the zeroth order mass of two states with the same k is degenerate and by definition the first-order correction to this mass is proportional to $1/m_Q$ as given by H_1 of Eq. (10) or by $H_1^{\alpha\beta}$ of Eq. (D10). To see Eq. (52) as a prediction, replacing E_X with the observed values M_X we obtain, to first order,

$$\frac{M_{B*}-M_B}{M_{D*}-M_D}=\frac{m_c}{m_b}=0.299, \tag{53}$$

which should be compared with the experimental value, 0.326. This discrepancy between the calculated and the observed comes from our calculation of B meson mass spectrum listed in Table V which give B and B^* meson masses slightly different values from the observed ones. Hold also equations similar to Eq. (52) for higher spin states with the same k quantum number because of the same reason given above.

(vii) The so-called $\overline{\Lambda}$ parameter can be calculated using the definition [3]

$$\overline{\Lambda}=\lim_{m_Q\to\infty}(E_H-m_Q)=M_0-m_Q=E_0^{-1}, \tag{54}$$

TABLE VI. B_s meson mass spectrum (first order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	5.399	$-2.92(\times 10^{-3})$	$1.84(\times 10^{-3})$	5.393	5.369
$^3S_1$ (1^-)		7.65	0.0936	5.440	-
$^3P_0$ (0^+)	5.701	0.923	1.74	5.716	-
‘‘$^3P_1$’’ (1^+)		10.3	0.100	5.760	-
‘‘$^1P_1$’’ (1^+)	5.748	8.35	0.0236	5.796	-
$^3P_2$ (2^+)		10.7	1.08×10^{-7}	5.809	-
$^3D_1$ (1^-)	5.814	197	0.0348	6.959	-
‘‘$^3D_2$’’ (2^-)		156	1.07×10^{-7}	6.719	-

TABLE VII. D meson mass spectrum (second order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	p_2/M_0	n_2/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	1.865	0.457($\times 10^{-4}$)	1.03($\times 10^{-2}$)	-1.86($\times 10^{-17}$)	-1.40($\times 10^{-2}$)	1.867	1.867
$^3S_1$ (1^-)		7.41	0.0540	-2.95×10^{-4}	0.209	2.008	2.008
$^3P_0$ (0^+)	2.319	2.33	0.828	3.44	0.689	2.408	-
“$^3P_1$” (1^+)		7.00	0.164	3.63×10^{-4}	-0.0107	2.486	2.422(?)
“$^1P_1$” (1^+)	2.205	8.22	0.0532	-3.82×10^{-4}	-0.0541	2.388	-
$^3P_2$ (2^+)		8.67	0.0156	-0.157	0.112	2.399	2.459
$^3D_1$ (1^-)	2.584	8.29	0.154	2.14×10^{-4}	-0.177	2.798	-
“$^3D_2$” (2^-)		8.13	0.0133	3.17	-0.134	2.791	-

where E_H, M_0, and m_Q are calculated heavy meson mass, the lowest degenerate bound state mass, and a heavy quark mass, respectively. Difference of M_0 and m_Q is nothing but the lowest leading eigenvalue, E_0^k, with $k=-1$ in our model. From Tables III and IV and $m_c=1.457$ listed in Table II, one obtains, to first order,

$$\overline{\Lambda_{u,d}}=M_{0D}-m_c=M_{0D*}-m_c=0.412 \text{ GeV}, \tag{55}$$

$$\overline{\Lambda_s}=M_{0D_s}-m_c=M_{0D_s^*}-m_c=0.529 \text{ GeV}, \tag{56}$$

and from Tables III and IV and $m_c=1.347$ listed in Table II, one obtains, to second order,

$$\overline{\Lambda_{u,d}}=M_{0D}-m_c=M_{0D*}-m_c=0.518 \text{ GeV}, \tag{57}$$

$$\overline{\Lambda_s}=M_{0D_s}-m_c=M_{0D_s^*}-m_c=0.629 \text{ GeV}, \tag{58}$$

where $M_{0D_{(s)}}$, $M_{0D^*_{(s)}}$ are the calculated lowest-order D meson mass defined by Eq. (54).

(viii) Parameters which give nonperturbative corrections to inclusive semileptonic B decays are defined as [17,18]

$$\lambda_1=\frac{1}{2m_Q}\langle H(v)|\overline{h_v}(iD)^2h_v|H(v)\rangle, \tag{59}$$

$$\lambda_2=\frac{1}{2m_Q}\left\langle H(v)\left|\overline{h_v}\frac{g}{2}\sigma_{\mu\nu}G^{\mu\nu}h_v\right|H(v)\right\rangle, \tag{60}$$

where h_v is the heavy quark field in the HQET with velocity v. $d_H=3, -1$ for pseudoscalar or vector mesons, respectively. Then the heavy meson mass can be expanded in terms of the heavy quark mass, λ_1, λ_2, and $\overline{\Lambda}$, as

$$E_H=m_Q+\overline{\Lambda}-\frac{\lambda_1+d_H\lambda_2}{2m_Q}+\cdots . \tag{61}$$

The first-order calculation in $1/m_Q$ makes $2\lambda_2$ equal to Eq. (52) and the λ_1 can be calculated using the above equation as

$$\lambda_1=2m_b(m_b+\overline{\Lambda_u}-\widetilde{E}_B)-3\lambda_2, \tag{62}$$

$$\lambda_2=\frac{m_b}{2}(\widetilde{E}_{B*}-\widetilde{E}_B), \tag{63}$$

where $\widetilde{E}_B$ and $\widetilde{E}_{B*}$ are the calculated B meson masses without the second-order corrections. The results are given by, to first order,

$$\lambda_1=-0.378 \text{ GeV}^2, \quad \lambda_2=0.112 \text{ GeV}^2, \tag{64}$$

and to second order,

$$\lambda_1=-0.238 \text{ GeV}^2, \quad \lambda_2=0.0255 \text{ GeV}^2. \tag{65}$$

Here we notice that although the first term in Eq. (62) is expected to be ~ 1, we find it to be small from Table V *to first order* and obtain the approximate relation

$$\lambda_1\sim -3\lambda_2. \tag{66}$$

These values should be compared with those in Ref. [19], which give $\overline{\Lambda_u}=0.39\pm 0.11$ GeV, $\lambda_1=-0.19\pm 0.10$ GeV^2, and $\lambda_2\simeq 0.12$ GeV^2.

(ix) Recently, it has been pointed out that the kinetic energy of heavy quark inside a heavy meson plays an important role in the determination of the ratios f_B/f_D, $(M_{B*}-M_B)/(M_{D*}-M_D)$, and $|V_{ub}/V_{cb}|$, in which use has been made the Gaussian form for the heavy meson wave

TABLE VIII. D_s meson mass spectrum (second order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	p_2/M_0	n_2/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	1.976	0.150($\times 10^{-2}$)	90.6($\times 10^{-4}$)	2.81($\times 10^{-17}$)	-1.60($\times 10^{-2}$)	1.965	1.969
$^3S_1$ (1^-)		7.76	4.65	-7.02×10^{-4}	0.243	2.133	2.112(?)
$^3P_0$ (0^+)	2.331	3.20	76.8	2.08	0.956	2.446	-
“$^3P_1$” (1^+)		8.12	3.87	2.20×10^{-3}	0.0361	2.527	2.535
“$^1P_1$” (1^+)	2.317	7.29	0.925	-2.22×10^{-3}	0.0229	2.482	-
$^3P_2$ (2^+)		8.31	2.96×10^{-8}	-5.98	-0.00166	2.509	2.574(?)
$^3D_1$ (1^-)	2.582	702	0.770	5.38×10^{-4}	-0.00632	2.072	-
“$^3D_2$” (2^-)		-4470	2.65×10^{-8}	212	0.000139	-113	-

TABLE IX. B meson mass spectrum (second order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	p_2/M_0	n_2/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	5.271	0.212($\times10^{-2}$)	10.3($\times10^{-4}$)	2.80($\times10^{-17}$)	-3.97($\times10^{-4}$)	5.286	5.279
$^3S_1$ (1^-)		0.862	0.541	-8.41×10^{-6}	0.593	5.317	5.325
$^3P_0$ (0^+)	5.725	0.387	9.50	-3.54	2.24	5.754	-
``$^3P_1$'' (1^+)		0.965	1.89	1.18×10^{-5}	-0.0347	5.782	-
``$^1P_1$'' (1^+)	5.611	1.08	0.593	-1.21×10^{-5}	0.171	5.672	-
$^3P_2$ (2^+)		1.23	0.174	-1.06	0.352	5.680	-
$^3D_1$ (1^-)	5.990	1.18	1.88	7.40×10^{-6}	-0.614	6.061	-
``$^3D_2$'' (2^-)		1.28	0.163	-6.48	-0.465	6.066	-

function and has been adopted the so-called Cornell potential, the same as ours [20]. They have derived the relation of these physical quantities in terms of the Fermi momentum, p_F, introduced in [21] in which p_F is related to a heavy quark recoil momentum, $\vec{p}$, by

$$\langle \vec{p}^{\,2} \rangle = \int d^3p\ \vec{p}^{\,2}\ \phi(\vec{p}\,) = \tfrac{3}{2}\,p_F^2, \tag{67}$$

where the momentum probability distribution function is given by

$$\phi(\vec{p}\,) = \left(\frac{2}{\sqrt{\pi}p_F}\right)^3 e^{-\vec{p}^{\,2}/p_F^2}. \tag{68}$$

They calculated the left-hand side (LHS) of Eq. (67) to obtain p_F by using the Gaussian form of the wave function and then derived the relations between physical quantities and this p_F [20]. We have the radial wave function given by Eq. (45) different from a Gaussian one and hence should have relations among physical quantities and our parameters, a, b, α_s, and m_c, independent of p_F and hence we may calculate the LHS of Eq. (67) to check if our calculation gives the value similar to other calculations. Our value of the LHS of Eq. (67) gives, for $\langle \vec{p}^{\,2} \rangle$ of the B meson to first order,

$$\langle \vec{p}^{\,2} \rangle = 0.560\ \ {\rm GeV}^2, \tag{69}$$

and the second order gives $\langle \vec{p}^{\,2} \rangle = 0.562$ GeV^2, which should be compared with the latest values $p_F = 0.5-0.6$ GeV calculated in [20] which correspond to $\langle \vec{p}^{\,2} \rangle = 0.375-0.540$ GeV^2.

(x) When one takes an overall look at the calculated masses, the negative component contributions, n_i/M_0, are relatively large for both scalar states, $0^\pm$, at the first as well as second order even though they become very small for higher spin states. Positive components constantly contribute to all states. When one compares the first-order with the second-order calculations, one cannot conclude that the second order is better than the first as a whole although higher spin states of D and B are largely improved at the second order. This conclusion may be also supported by the comparison of the first- and second-order calculations of the parameters, λ_1, λ_2, and $\overline{\Lambda}$ with other calculations [19]. In order to incorporate the second-order effects properly, one may need to introduce a different potential and/or method from ours as mentioned in (iv) in this section.

We have used the following algorithms to calculate numerically the heavy meson masses, Gauss-Hermite quadrature to evaluate integrals, and the tridiagonal QL implicit method to determine the eigenvalues and eigenvectors of a finite dimensional real matrix [22].

V. COMMENTS AND DISCUSSIONS

In this paper, we have calculated heavy meson masses, $D_{(s)}$, $D^*_{(s)}$, $B_{(s)}$, $B^*_{(s)}$, etc., based on the formulation proposed before [4], which develops the perturbation potential theory in terms of inverse power of a heavy quark mass. The first and second-order calculations of masses are in good agreement with the experimental data except for the higher spin states even though the second-order calculation does not much improve the first order. The first-order calculation of the HQET quantities, λ_1, λ_2, and $\overline{\Lambda}$, are also in good agreement with the other calculations [19]. A new study on the

TABLE X. B_s meson mass spectrum (second order).

State (J^P)	M_0	p_1/M_0	n_1/M_0	p_2/M_0	n_2/M_0	$M_{\rm calc}$	$M_{\rm obs}$
$^1S_0$ (0^-)	5.382	0.161($\times10^{-2}$)	9.43($\times10^{-4}$)	-7.46($\times10^{-17}$)	-4.72($\times10^{-4}$)	5.393	5.369
$^3S_1$ (1^-)		0.882	0.483	-2.07×10^{-5}	0.717	5.430	-
$^3P_0$ (0^+)	5.739	0.505	8.84	3.12×10^{-4}	3.12	5.773	-
``$^3P_1$'' (1^+)		1.11	0.446	7.19×10^{-5}	0.118	5.801	-
``$^1P_1$'' (1^+)	5.723	1.03	0.106	-7.21×10^{-5}	0.0743	5.782	-
$^3P_2$ (2^+)		1.19	3.39×10^{-9}	-3.78	-0.00540	5.791	-
$^3D_1$ (1^-)	5.988	43.9	0.0940	1.86×10^{-5}	-0.0219	8.618	-
``$^3D_2$'' (2^-)		-136	3.24×10^{-9}	-2.06	4.82×10^{-8}	-2.174	-

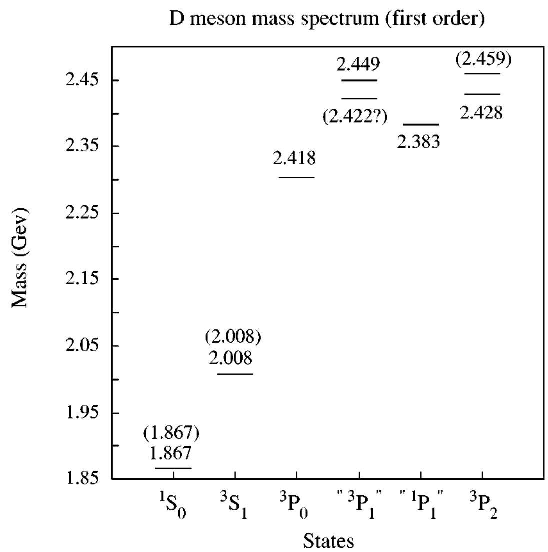

FIG. 2. The first-order plot of D meson masses. Values in the brackets are the observed values.

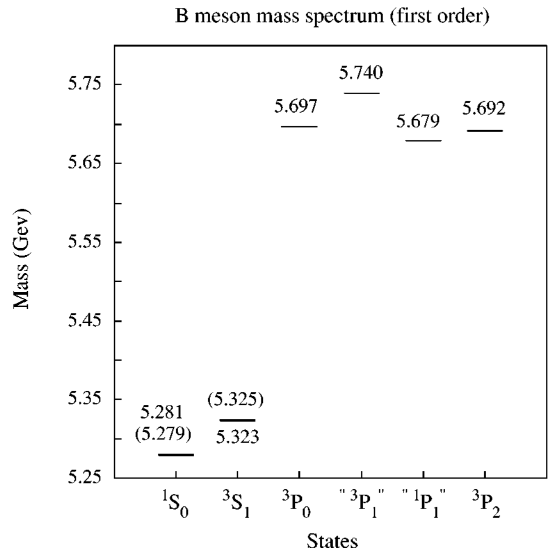

FIG. 4. The first-order plot of B meson masses. Values in the brackets are the observed values.

HQET introduced the Fermi momentum, p_F, to obtain other physical quantities [20]. Although we have not had p_F in our mind at the begining of this study, the obtained value given by Eq. (69) is in good agreement with what they have obtained [20].

We have also found a new symmetry already mentioned in the paper [4] and realized by the operator, Eq. (19),

$$-\beta_q(\vec{\Sigma}_q\cdot\vec{\ell}+1),$$

which is always present when one considers a centrally symmetric potential model for two particles or when one takes a rest frame limit of a general relativistic form of the wave function and is related to a light quark spin structure, i.e., $y_{j\ m}^{k}(\Omega)$. That is, this is quite a general symmetry, not a special feature peculiar to our potential model.

One can easily see degeneracy among the lowest lying pseudoscalar and vector states as follows. Define

$$|P\rangle=U_c^{-1}(0\quad\Psi_{00}^{-1}),\quad |V,\lambda\rangle=U_c^{-1}(0\quad\Psi_{1\lambda}^{-1}),\qquad(70)$$

where the inverse of the charge conjugate operator, U_c^{-1}, is defined in Appendix A. Equations (A2), Ψ_{jm}^{k} is an eigenfunction obtained in the last chapter. The explicit forms of these wave functions are given in Appendix C, Eqs. (C28) and (C29), and the quantum number k can take only $\pm j$, or $\pm(j+1)$. Assigning these states to D mesons, one can have

$$|P\rangle=|D^{\pm}\rangle,\ \text{or}\ |D^0\rangle,\quad |V,\lambda\rangle=|D^*\rangle.\qquad(71)$$

Since these states have the same quantum number $k=-1$, these have the same masses as well as the same wave functions up to the zeroth order calculation in $1/m_Q$. That is, the degeneracy among these states is simply the result of the

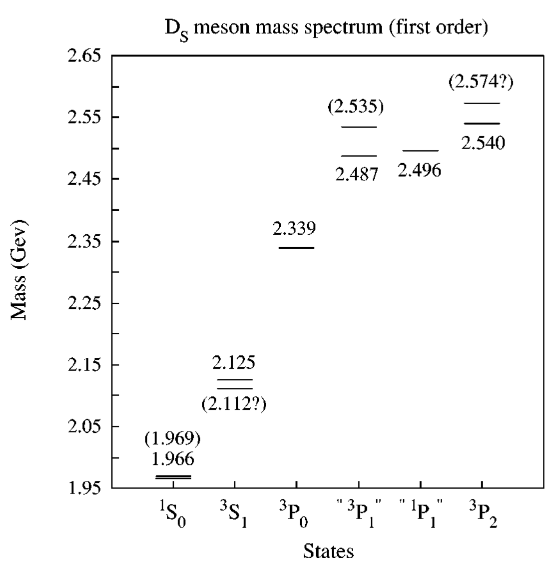

FIG. 3. The first-order plot of D_s meson masses. Values in the brackets are the observed values.

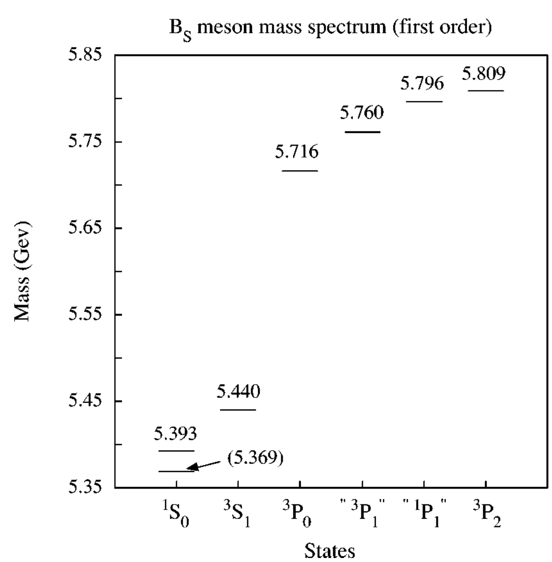

FIG. 5. The first-order plot of B_s meson masses. Values in the brackets are the observed values.

TABLE XI. States classified by various quantum numbers.

k	-1	-1	1	1	-2	-2	2	2
j	0	1	0	1	1	2	1	2
J^P	0^-	1^-	0^+	1^+	1^+	2^+	1^-	2^-
$^{2S+1}L_J$	$^1S_0$	$^3S_1$	$^3P_0$	$^3P_1,\ ^1P_1$	$^1P_1,\ ^3P_1$	$^3P_2$	$^3D_1$	$^3D_2,\ ^1D_2$

special property of the eigenvalue equation. Higher-order corrections can be obtained by developing perturbation of energy and wave function for each state in terms of $\Lambda_{\rm QCD}/m_Q$ as given by Eqs. (14) and (15):

$$\tilde{E}\equiv E-m_Q=E_0^{\prime}+E_1^{\prime}+E_2^{\prime}+\cdots\ ,$$

$$\psi_{\rm FWT}=\psi_0^{\prime}+\psi_1^{\prime}+\psi_2^{\prime}+\cdots\ .$$

Finally we would like to discuss qualitative features of form factors/ Isgur-Wise functions. Let us think about calculating form factors for the semileptonic decay of B meson into D. Taking a simple form for the lowest lying wave function both for B and D as

$$\Psi^{1S}\sim e^{-b^2\ r^2/2},$$

where a parameter b is determined by a variational principle, $\delta(\Psi^{1S\ \dagger}H\Psi^{1S})=0$. Then form factors are given by

$$F(q^2)\sim\exp[{\rm const}\times\tilde{E}^2(q^2-q^2_{\rm max})],\ \ \text{or}\ \ \xi(\omega)\sim\exp[{\rm const}\times\tilde{E}^2(\omega-1)],$$

where

$$q^2=(p_B-p_D)^2,\quad \omega=v_B\cdot v_D,$$

$$q^2_{\rm max}=(m_B-m_D)^2\leftrightarrow\omega_{\rm max}=1,$$

with $v^{\mu}_{B,D}$ being four-velocity of B and/or D meson. This means behavior of form factors strongly depends on an eigenvalue, $\tilde{E}=E-m_Q$ of the eigenvalue equation, Eq. (23), which is often called ''inertia'' parameter $\overline{\Lambda}_q$ when $m_Q\to\infty$. This quantity $\tilde{E}$ does not depend on any heavy quark properties at the zeroth order. This result also means that the slope at the origin of the Isgur-Wise function includes the term proportional to $\tilde{E}^2$. The constant term ($-1/4$ like the Bjorken limit [23]) for this slope should be given by a kinematical factor multiplied with the above expression.

To conclude, although there have been various relativistic bound state equations proposed so far, nobody has yet determined what the most preferable is. We believe that our approach presented here must be a promising candidate.

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APPENDIX A: SCHRÖDINGER EQUATION

In order to derive Eq. (4) or Eq. (5), we need to calculate the expectation value

$$\langle\psi|(\mathcal{H}_0+\mathcal{H}_{\rm int}-E)|\psi\rangle \tag{A1}$$

by using the equal-time anticommutation relations among quark fields,

$$\{q^c_\alpha(x),\ q^{c\,\dagger}_\beta(x')\}_{x_0=x_0'}=\delta_{\alpha\,\beta}\delta^3(\vec{x}-\vec{x}\,'),$$

$$\{Q_\alpha(x),\ Q^\dagger_\beta(x')\}_{x_0=x_0'}=\delta_{\alpha\,\beta}\delta^3(\vec{x}-\vec{x}\,').$$

Since the wave function, $\psi_{\alpha\,\beta}(x-y)$ defined in Eq. (3), has a constant normalization, what we need to do is to variate Eq. (A1) in terms of $\psi^*_{\alpha\,\beta}(x-y)$ and to set it equal to zero. Then we can easily obtain Eq. (4) with the effective Hamiltonian given by Eq. (7). In the course of this derivation, it appears to be clear that $\vec{p}$ and $\vec{p}\,'$ operates on the initial and final wave functions, respectively, while $\vec{q}$ only on potentials.

To derive the FWT and charge conjugate transformed Schrödinger equation given by Eq. (5), we have used the following definitions:

$$H_{\rm FWT}=U_cU_{\rm FWT}(p_Q')HU^{-1}_{\rm FWT}(p_Q)U_c^{-1},$$

$$\psi_{\rm FWT}=U_cU_{\rm FWT}(p_Q)\psi, \tag{A2a}$$

$$U_{\rm FWT}(p)=\exp(W(p)\vec{\gamma}_Q\cdot\hat{\vec{p}})=\cos W+\vec{\gamma}_Q\cdot\hat{\vec{p}}\ \sin W, \tag{A2b}$$

$$\hat{\vec{p}}=\frac{\vec{p}}{p},\quad \tan W(p)=\frac{p}{m_Q+E},\quad E=\sqrt{\vec{p}^{\,2}+m_Q^2}, \tag{A2c}$$

$$U_c=i\ \gamma^0_Q\gamma^2_Q=-U_c^{-1}. \tag{A2d}$$

Note that the argument of the FWT transformation, $U_{\rm FWT}$, operating on a Hamiltonian from left is different from the right-operating one, since an outgoing momentum, $\vec{p}_Q\,'$, is different from an incoming one, $\vec{p}_Q$. However, here in our study we work in a configuration space which means momenta are nothing, but the derivative operators and when we write them differently, for instance as $\vec{p}_Q$ and $\vec{p}_Q'$, their expressions are reminders of their momentum representation. Hence although the arguments of $U_{\rm FWT}$ and $U^{-1}_{\rm FWT}$ look different $\vec{p}_Q$ and $\vec{p}_Q'$ are the same derivative operator, $-i\vec{\nabla}$. Here the difference between $\vec{p}_Q$ and $\vec{p}_Q'$ is $\vec{q}$ which operates only on potentials and gives nonvanishing results. The FWT transformation is introduced so that a heavy quark inside a heavy meson be treated as a nonrelativistic color source. The charge conjugation operator, U_c, is introduced to make the wave function, $U_c\psi$, a true bi-spinor, i.e., gamma matrices of a light anti-quark are multiplied from left while those of a heavy quark from right, which is expressed by using a notation $\otimes$.

To derive Eqs. (10), we need to first expand $H_{\rm FWT}$ in $1/m_Q$ and then take into account the following properties of a charge conjugation operator, $U_c = i\gamma_Q^0\gamma_Q^2$, to obtain the final expressions

$$U_c^{-1}\gamma_Q^{\mu}\,U_c = -\gamma_Q^{\mu T}, \tag{A3}$$

i.e.,

$$U_c\beta_Q U_c^{-1} = -\beta_Q{}^T,$$

$$U_c\vec{\alpha}_Q U_c^{-1} = -\vec{\alpha}_Q{}^T, \quad U_c\vec{\Sigma}_Q U_c^{-1} = -\vec{\Sigma}_Q{}^T,$$

$$U_c\vec{\gamma}_Q U_c^{-1} = -\vec{\gamma}_Q{}^T, \quad U_c\gamma_Q^5 U_c^{-1} = -\gamma_Q^{5\,T}, \tag{A4}$$

where a superscript T means its transposed matrix. Hence the projection operators are given by

$$U_c\frac{1\pm\beta_Q}{2}U_c^{-1} = \frac{1\mp\beta_Q^T}{2}. \tag{A5}$$

APPENDIX B: DERIVATION OF PERTURBATION

In this Appendix we will follow the paper [4] to derive perturbative Schrödinger equation for a Hamiltonian given by Eq. (7) for consistency. Following that paper, we will give an equation at each order by using the explicit interaction terms given by Eqs. (10). Here we quote the same equations given in the former sections for clarification of derivation. The fundamental Schrödinger equation is given by

$$(H_{\rm FWT}-m_Q)\otimes\psi_{\rm FWT} = \tilde{E}\psi_{\rm FWT}, \tag{B1}$$

and expansion of each quantity in $1/m_Q$ is given by

$$H_{\rm FWT}-m_Q = H_{-1}+H_0+H_1+H_2+\cdots, \tag{B2a}$$

$$\tilde{E} = E_0^{\ell}+E_1^{\ell}+E_2^{\ell}+\cdots, \tag{B2b}$$

$$\psi_{\rm FWT} = \psi_0^{\ell}+\psi_1^{\ell}+\psi_2^{\ell}+\cdots. \tag{B2c}$$

With a help of projection operators defined by

$$\Lambda_{\pm} = \frac{1\pm\beta_Q}{2}, \tag{B3}$$

we will derive the Schrödinger equation at each order.

1. −1st order

From Eqs. (B1) and (B2), the -1st-order Schrödinger equation in $1/m_Q$ is given by

$$-2m_Q\Lambda_+\otimes\psi_0^{\ell} = 0, \tag{B4}$$

which means

$$\psi_0^{\ell} = \Lambda_-\otimes\psi_0^{\ell}. \tag{B5}$$

Remember that matrices of a heavy quark should be multiplied from right. That is, the zeroth-order wave function has only a positive component of the heavy quark sector and is given by

$$\psi_0^{\ell} = \Psi_{\ell}^{+} = \begin{pmatrix} 0 & f_{\ell}(\vec{r}) \\ 0 & g_{\ell}(\vec{r}) \end{pmatrix}, \tag{B6}$$

where f_{ℓ} and g_{ℓ} are 2 by 2 matrices. More explicit form of this wave function is given in Appendix C.

2. Zeroth order

The zeroth-order equation is given by

$$-2m_Q\Lambda_+\otimes\psi_1^{\ell}+H_0\otimes\psi_0^{\ell} = E_0^{\ell}\psi_0^{\ell}. \tag{B7}$$

Multiplying projection operators, $\Lambda_{\mp}$, from right, respectively, we obtain

$$H_0\Lambda_-\otimes\psi_0^{\ell} = E_0^{\ell}\psi_0^{\ell}, \tag{B8}$$

$$-2m_Q\Lambda_+\otimes\psi_1^{\ell}+H_0\Lambda_+\otimes\psi_0^{\ell} = 0, \tag{B9}$$

whose explicit forms are given by Eqs. (22) and (23), where use has been made of

$$\Lambda_+\otimes\psi_0^{\ell} = 0.$$

Detailed analysis of Eq. (B8) is given in Appendix C. When one expands Λ_+ components of ψ_1^{ℓ} in terms of the eigenfunctions,

$$\Psi_{\ell}^{-} = \begin{pmatrix} f_{\ell}(\vec{r}) & 0 \\ g_{\ell}(\vec{r}) & 0 \end{pmatrix}, \tag{B10}$$

like

$$\Lambda_+\otimes\psi_1^{\ell} = \sum_{\ell'} c_{1-}^{\ell\,\ell'}\Psi_{\ell'}^{-}, \tag{B11}$$

one can solve Eq. (B9) to obtain coefficients, $c_{1-}^{\ell\,\ell'}$, as

$$c_{1-}^{\ell\,\ell'} = \frac{1}{2m_Q}\langle\Psi_{\ell'}^{-}|\Lambda_-H_0\Lambda_+|\Psi_{\ell}^{+}\rangle, \tag{B12}$$

whose explicit form is given by Eq. (26). Here in this paper the eigenfunctions, $\Psi_{\ell}^{\pm}$ are normalized to be 1,

$$\langle\Psi_{\ell}^{\alpha}|\Psi_{\ell'}^{\beta}\rangle = \delta_{\ell\,\ell'}\delta^{\alpha\,\beta} \quad \text{for } \alpha,\ \beta=+-. \tag{B13}$$

The inner product like $\langle\Psi_{\ell}^{\alpha}|O|\Psi_{\ell'}^{\beta}\rangle$ is defined by Eq. (27).

3. 1st order

The 1st-order equation is given by

$$-2m_Q\Lambda_+\otimes\psi_2^{\ell}+H_0\otimes\psi_1^{\ell}+H_1\otimes\psi_0^{\ell} = E_0^{\ell}\psi_1^{\ell}+E_1^{\ell}\psi_0^{\ell}. \tag{B14}$$

As in the above case, multiplying projection operators from right, we obtain

$$H_0\Lambda_-\otimes\psi_1^\ell+H_1\Lambda_-\otimes\psi_0^\ell=E_0^\ell\Lambda_-\otimes\psi_1^\ell+E_1^\ell\psi_0^\ell, \tag{B15}$$

$$-2m_Q\Lambda_+\otimes\psi_2^\ell+H_0\Lambda_+\otimes\psi_1^\ell+H_1\Lambda_+\otimes\psi_0^\ell=E_0^\ell\Lambda_+\otimes\psi_1^\ell. \tag{B16}$$

The first equation, Eq. (B15), can be solved like in the ordinary perturbation theory of quantum mechanics. First expanding ψ_1^k in terms of $\Psi_k^\pm$ as

$$\psi_1^\ell=\sum_{\ell'}\left(c_{1+}^{\ell\ell'}\Psi_{\ell'}^{+}+c_{1-}^{\ell\ell'}\Psi_{\ell'}^{-}\right), \tag{B17}$$

and next taking the inner product of the whole Eq. (B15) with $\langle\Psi_k^+|$, one obtains

$$E_0^k\,c_{1+}^{\ell k}+\sum_{\ell'}c_{1-}^{\ell\ell'}\langle\Psi_k^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_k^+|\Lambda_-H_1\Lambda_-|\Psi_\ell^+\rangle=E_0^\ell\,c_{1+}^{\ell k}+E_1^k\,\delta_{\ell k}, \tag{B18}$$

where we have used the orthogonality condition, Eq. (B13), and the lowest Schrödinger equation, Eq. (B8), to obtain the first term of the LHS and two terms of the RHS of Eq. (B18). When one sets $k=\ell$ in Eq. (B18), one obtains

$$E_1^\ell=\sum_{\ell'}c_{1-}^{\ell\ell'}\langle\Psi_\ell^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_\ell^+|\Lambda_-H_1\Lambda_-|\Psi_\ell^+\rangle, \tag{B19}$$

which gives the first-order perturbation correction to the mass when one calculates matrix elements of the RHS among eigenfunctions, $\Psi_k^\pm$, like in the ordinary perturbation of quantum mechanics. When one sets $k\neq\ell$ in Eq. (B18), one obtains

$$c_{1+}^{\ell k}=\frac{1}{E_0^\ell-E_0^k}\left[\sum_{\ell'}c_{1-}^{\ell\ell'}\langle\Psi_k^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_k^+|\Lambda_-H_1\Lambda_-|\Psi_\ell^+\rangle\right]. \tag{B20}$$

The coefficient c_{1+}^{kk} cannot be determined by the above equation, which can be derived by calculating a normalization of the total wave function up to the first order,

$$\langle\psi^\ell|\psi^{\ell'}\rangle=\delta_{\ell\ell'}, \tag{B21}$$

giving

$$c_{1+}^{kk}=0. \tag{B22}$$

This completes the solution for ψ_1^ℓ since $\Lambda_-\psi_1^\ell$, or $c_{1-}^{\ell\ell'}$, is obtained in the last chapter, Eq. (B12). The definition of the normalization, Eq. (B21), is already mentioned in the main text below Eq. (34) and hence we will not repeat that argument here. This way of solving Eq. (B15) is unique and we will use this method below to solve similar equations appearing in Sec. III D as well.

Equation (B16) gives a Λ_+ component of ψ_2^ℓ as in the case of $\Lambda_+\otimes\psi_1^\ell$ in the Sec. III B, i.e., setting

$$\Lambda_+\otimes\psi_2^\ell=\sum_{\ell'}c_{2-}^{\ell\ell'}\Psi_{\ell'}^-, \tag{B23}$$

one obtains coefficients, $c_{2-}^{\ell\ell'}$, as

$$c_{2-}^{\ell\ell'}=\frac{1}{2m_Q}\langle\Psi_{\ell'}^-|[(H_0-E_0^\ell)\Lambda_+\otimes\psi_1^\ell+H_1\Lambda_+\otimes\psi_0^\ell]\rangle. \tag{B24}$$

4. 2nd order

The 2nd-order equation is given by

$$-2m_Q\Lambda_+\otimes\psi_3^\ell+H_0\otimes\psi_2^\ell+H_1\otimes\psi_1^\ell+H_2\otimes\psi_0^\ell=E_0^\ell\psi_2^\ell+E_1^\ell\psi_1^\ell+E_2^\ell\psi_0^\ell. \tag{B25}$$

As in the above cases, multiplying projection operators from right we obtain

$$H_0\Lambda_-\otimes\psi_2^\ell+H_1\Lambda_-\otimes\psi_1^\ell+H_2\Lambda_-\otimes\psi_0^\ell=E_0^\ell\Lambda_-\otimes\psi_2^\ell+E_1^\ell\Lambda_-\otimes\psi_1^\ell+E_2^\ell\psi_0^\ell, \tag{B26}$$

$$-2m_Q\Lambda_+\otimes\psi_3^\ell+H_0\Lambda_+\otimes\psi_2^\ell+H_1\Lambda_+\otimes\psi_1^\ell+H_2\Lambda_+\otimes\psi_0^\ell=E_0^\ell\Lambda_+\otimes\psi_2^\ell+E_1^\ell\Lambda_+\otimes\psi_1^\ell. \tag{B27}$$

Again to solve the first equation, Eq. (B26), first expanding ψ_2^ℓ in terms of $\Psi_\ell^\pm$ as

$$\psi_2^\ell=\sum_{\ell}\left(c_{2+}^{\ell\ell'}\Psi_{\ell'}^{+}+c_{2-}^{\ell\ell'}\Psi_{\ell'}^{-}\right), \tag{B28}$$

and next taking the inner product of the whole Eq. (B26) with $\langle\Psi_k^+|$, one obtains

$$E_0^k\,c_{2+}^{\ell k}+\sum_{\ell'}c_{2-}^{\ell\ell'}\langle\Psi_k^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_k^+|H_1\Lambda_-\otimes\psi_1^\ell\rangle+\langle\Psi_k^+|\Lambda_-H_2\Lambda_-|\Psi_\ell^+\rangle=E_0^\ell\,c_{2+}^{\ell k}+E_1^\ell\,c_{1+}^{\ell k}+E_2^\ell\,\delta_{\ell k}, \tag{B29}$$

where we have used the orthogonality condition, Eq. (B13), and the lowest Schrödinger equation, Eq. (B8), to obtain the first term of the LHS and three terms of the RHS of Eq. (B29). When one sets $k=\ell$ in Eq. (B29), since $c_{1+}^{\ell\ell}=0$ one obtains

$$E_2^\ell=\sum_{\ell'}c_{2-}^{\ell\ell'}\langle\Psi_\ell^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle+\langle\Psi_\ell^+|H_1\Lambda_-\otimes\psi_1^\ell\rangle+\langle\Psi_\ell^+|\Lambda_-H_2\Lambda_-|\Psi_\ell^+\rangle, \tag{B30}$$

which gives the second-order perturbation corrections to the mass when one calculates matrix elements of the RHS among eigenfunctions. When one sets $k\neq\ell$ in Eq. (B29), one obtains

$$c_{2+}^{\ell\,k}=\frac{1}{E_0^\ell-E_0^k}\Bigg[\sum_{\ell'} c_{2-}^{\ell\,\ell'}\langle\Psi_k^+|\Lambda_+H_0\Lambda_-|\Psi_{\ell'}^-\rangle + \langle\Psi_k^+|H_1\Lambda_-\otimes\psi_1^\ell\rangle+\langle\Psi_k^+|\Lambda_-H_2\Lambda_-|\Psi_\ell^+\rangle - E_1^\ell\, c_{1+}^{\ell\,k}\Bigg]. \tag{B31}$$

The coefficient $c_{2+}^{k\,k}$ can be derived by calculating a normalization of the total wave function up to the second order, Eq. (B21), which gives

$$c_{2+}^{k\,k}=-\frac{1}{2}\sum_\ell (|c_{1+}^{k\,\ell}|^2+|c_{1-}^{k\,\ell}|^2). \tag{B32}$$

This completes the solution for ψ_2^k since $\Lambda_-\psi_2^k$, or $c_{2-}^{\ell\,\ell'}$, is obtained in the last chapter, Eq. (B24).

Although we do not use, Eq. (B27) gives a Λ_+ component of ψ_3^ℓ as in the cases of $\Lambda_+\otimes\psi_1^\ell$ and $\Lambda_+\otimes\psi_2^\ell$ given in the Secs. III B and III C, i.e., setting

$$\Lambda_+\otimes\psi_3^\ell=\sum_{\ell'} c_{3-}^{\ell\,\ell'}\Psi_{\ell'}^-, \tag{B33}$$

one obtains coefficients, $c_{3-}^{\ell\,\ell'}$, as given by Eq. (42).

APPENDIX C: ZEROTH-ORDER SOLUTION

There have been a couple of trials to solve Eq. (22) [11,12,7]. In order to solve the lowest nontrivial eigenvalue equation given by Eq. (22), i.e.,

$$[\vec{\alpha}_q\cdot\vec{p}+\beta_q(m_q+S)+V]\otimes\psi_0^\ell=E_0^\ell\psi_0^\ell, \tag{C1}$$

we summarize and refresh the previous results. First we need to introduce the so-called vector spherical harmonics which are defined by

$$\vec{Y}_{j\,m}^{(\mathrm{L})}=-\vec{n}\;Y_j^m, \tag{C2}$$

$$\vec{Y}_{j\,m}^{(\mathrm{E})}=\frac{r}{\sqrt{j(j+1)}}\vec{\nabla}Y_j^m, \tag{C3}$$

$$\vec{Y}_{j\,m}^{(\mathrm{M})}=-i\vec{n}\times\vec{Y}_{j\,m}^{(\mathrm{E})}=\frac{-ir}{\sqrt{j(j+1)}}\vec{n}\times\vec{\nabla}Y_j^m, \tag{C4}$$

where Y_j^m are spherical polynomials (or surface harmonics). These vector spherical harmonics satisfy the orthogonality condition:

$$\int d\Omega\vec{Y}_{j\,m}^{(\mathrm{A})}(\Omega)^\dagger\cdot\vec{Y}_{j'\,m'}^{(\mathrm{B})}(\Omega)=\delta_{j\,j'}\delta_{m\,m'}\delta^{\mathrm{A\,B}},$$

where $d\Omega=\sin\theta d\theta d\phi$. This is nothing, but a set of eigenfunctions for a spin-1 particle. In this paper we need their spinor representation and also need to unitary-transform them to obtain the functions, $y_{j\,m}^k$, as

$$\begin{pmatrix} y_{j\,m}^{-(j+1)} \\ y_{j\,m}^{j}\end{pmatrix}=U\begin{pmatrix} Y_j^m \\ \vec{\sigma}\cdot\vec{Y}_{j\,m}^{(\mathrm{M})}\end{pmatrix},\quad \begin{pmatrix} y_{j\,m}^{j+1} \\ y_{j\,m}^{-j}\end{pmatrix}=U\begin{pmatrix} \vec{\sigma}\cdot\vec{Y}_{j\,m}^{(\mathrm{L})} \\ \vec{\sigma}\cdot\vec{Y}_{j\,m}^{(\mathrm{E})}\end{pmatrix}, \tag{C5}$$

where to diagonalize the leading Hamiltonian in the k space the orthogonal matrix U is introduced,

$$U=\frac{1}{\sqrt{2j+1}}\begin{pmatrix}\sqrt{j+1} & \sqrt{j}\\ -\sqrt{j} & \sqrt{j+1}\end{pmatrix}. \tag{C6}$$

Here the values of the new quantum number k are distinguished by the operator given by Eq. (19). $\vec{Y}_{j\,m}^{(\mathrm{A})}$ (A=L, M, E) are eigenfunctions of $\vec{j}^2$ and j_z, having the eigenvalues, $j(j+1)$ and m. Parities are assigned as $(-)^{j+1},(-)^j,(-)^{j+1}$ for A=L, M, E, respectively, and Y_j^m has a parity $(-)^j$. Here

$$\vec{j}=\vec{\ell}+\vec{s}_q+\vec{s}_Q, \tag{C7}$$

and $\vec{s}_q=\vec{\sigma}_q/2$ and $\vec{s}_Q=\vec{\sigma}_Q/2$ are spin operators of light antiquark and heavy quark, respectively. $y_{j\,m}^k$ are 2×2-matrix eigenfunctions of three operators, $\vec{j}^{\,2}$, j_z, and $\vec{\sigma}\cdot\vec{\ell}$ with eigenvalues, $j(j+1)$, m, and $-(k+1)$, and satisfy

$$\frac{1}{2}\mathrm{tr}\left(\int d\Omega y_{j'm'}^{k'\,\dagger}y_{jm}^k\right)=\delta^{k\,k'}\delta_{j\,j'}\delta_{m\,m'}. \tag{C8}$$

Here the quantum number k can take only values, $\pm j$, or $\pm(j+1)$, and $\neq0$ since $\vec{Y}_{0\,0}^{(\mathrm{M})}$ does not exit. The eigenfunction of the zeroth order Hamiltonian depends on three quantum numbers, j, m, and k as described next. Functions, $\vec{Y}_{j\,m}^{(\mathrm{A})}$ and $y_{j\,m}^k$, have the following correspondence to those defined in Ref. [7] as

$$y_{j\,m}^{-(j+1)}\leftrightarrow y_1^{j\,m},\quad y_{j\,m}^{j}\leftrightarrow y_2^{j\,m},$$
$$y_{j\,m}^{j+1}\leftrightarrow y_+^{j\,m},\quad y_{j\,m}^{-j}\leftrightarrow y_-^{j\,m}, \tag{C9}$$

and

$$\vec{Y}_{jm}^{(\mathrm{L})}\leftrightarrow\vec{Y}_{j\,(-)}^m,\quad \vec{Y}_{j\,m}^{(\mathrm{E})}\leftrightarrow\vec{Y}_{j\,(+)}^m,$$
$$\vec{Y}_{j\,m}^{(\mathrm{M})}\leftrightarrow\vec{X}_{j\,j}^m. \tag{C10}$$

The explicit expressions of the first few $y_{j\,m}^k$ are given by

$$y_{00}^{-1}=\frac{1}{\sqrt{4\pi}},\quad y_{00}^1=-\frac{1}{\sqrt{4\pi}}(\vec{\sigma}\cdot\vec{n}), \tag{C11}$$

$$y_{1m}^{-1}=\frac{i}{\sqrt{4\pi}}\sigma^m,\quad y_{1m}^1=-\frac{i}{\sqrt{4\pi}}(\vec{\sigma}\cdot\vec{n})\sigma^m, \tag{C12}$$

where we have used

$$Y_0^0=\frac{1}{\sqrt{4\pi}},\quad Y_1^0=i\sqrt{\frac{3}{4\pi}}\cos\theta,$$

$$Y_1^{\pm} = \mp i \sqrt{\frac{3}{8\pi}} \sin\,\theta e^{\pm i\varphi}. \tag{C13}$$

In order to solve Eq. (C1), one can in general assume the form of the solution as

$$\psi_0^{\ell} = \Psi_{\ell}^{+} = (0 \quad \Psi_{j\,m}^{k}(\vec{r})), \tag{C14}$$

where ℓ stands for all the quantum numbers, j, m, and k and

$$\Psi_{j\,m}^{k}(\vec{r}) = \begin{pmatrix} F_k(\vec{r}) \\ G_k(\vec{r}) \end{pmatrix} \; y_{j\,m}^{k}(\Omega). \tag{C15}$$

Since the effective lowest order Hamiltonian does not include the heavy quark matrices, one can exclude the symbol $\otimes$ from Eq. (C1). The form of a radial wave function is in general given by

$$\begin{pmatrix} F_k(\vec{r}) \\ G_k(\vec{r}) \end{pmatrix} = \begin{pmatrix} f_{1\,k}(r) - f_{2\,k}(r)(\vec{\sigma}\cdot\vec{n}) \\ g_{1\,k}(r) - g_{2\,k}(r)(\vec{\sigma}\cdot\vec{n}) \end{pmatrix}. \tag{C16}$$

Substituting this into Eq. (C1), multiplying $y_{j\,m}^{k\,\dagger}$ from left, and using the orthogonality equation for $y_{j\,m}^{k}$, Eq. (C8), the simultaneous equations for $f_{i\,k}$ and $g_{i\,k}$ are obtained and after some calculations the final form of the wave function is determined to be either

$$\Psi_{j\,m}^{k} = \begin{pmatrix} f_{1\,k}(r) \\ -g_{2\,k}(r)(\vec{\sigma}\cdot\vec{n}) \end{pmatrix} y_{j\,m}^{k} = \begin{pmatrix} f_{1\,k}(r)\; y_{j\,m}^{k} \\ g_{2\,k}(r)\; y_{j\,m}^{-k} \end{pmatrix}, \tag{C17}$$

or

$$\Psi_{j\,m}^{k} = \begin{pmatrix} -f_{2\,k}(r)(\vec{\sigma}\cdot\vec{n}) \\ g_{1\,k}(r) \end{pmatrix} \; y_{j\,m}^{k} = \begin{pmatrix} f_{2\,k}(r)\; y_{j\,m}^{-k} \\ g_{1\,k}(r)\; y_{j\,m}^{k} \end{pmatrix} = \begin{pmatrix} f_{2\,k}(r) \\ -g_{1\,k}(r)(\vec{\sigma}\cdot\vec{n}) \end{pmatrix} \; y_{j\,m}^{-k}. \tag{C18}$$

Since Eq. (C18) assumes the same form as Eq. (C17), we generally define the eigenfunction, $\Psi_{j\,m}^{k}$, given by Eq. (C17). Then the reduced Schrödinger equation is given by

$$\left[i\left(\partial_r + \frac{1}{r}\right)\rho_1 + \frac{k}{r}\rho_2 + [m_q + S(r)]\rho_3 + V(r)\right]\Psi_k(r) = E_0^k\; \Psi_k(r), \tag{C19}$$

with

$$\Psi_k(r) \equiv \begin{pmatrix} f_{1\,k}(r) \\ g_{2\,k}(r) \end{pmatrix}. \tag{C20}$$

Here defined also are

$$\vec{\alpha}_q = \begin{pmatrix} 0 & \vec{\sigma}_q \\ \vec{\sigma}_q & 0 \end{pmatrix} = \rho_1\; \vec{\sigma}, \quad \beta_q = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \rho_3\; 1_{2\times 2}, \tag{C21}$$

$$\rho_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \rho_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{C22}$$

Finally introducing the unitary matrix,

$$R = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}, \quad R^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, \tag{C23}$$

one can transform eigenvalue equations as well as eigenfunctions into

$$\left\{ r\; R\left[i\left(\partial_r + \frac{1}{r}\right)\rho_1 + \frac{k}{r}\rho_2 + [m_q + S(r)]\rho_3 + V(r)\right] \frac{1}{r}\; R^{-1}\right\}\Phi_k(r) = E_0^k\; \Phi_k(r), \tag{C24}$$

or

$$\begin{pmatrix} m_q + S + V & -\partial_r + \frac{k}{r} \\ \partial_r + \frac{k}{r} & -m_q - S + V \end{pmatrix} \begin{pmatrix} u_k(r) \\ v_k(r) \end{pmatrix} = E_0^k \; \begin{pmatrix} u_k(r) \\ v_k(r) \end{pmatrix}, \tag{C25}$$

with

$$\Phi_k(r) \equiv \begin{pmatrix} u_k(r) \\ v_k(r) \end{pmatrix} = r\; R\; \Psi_k(r) = \begin{pmatrix} r\; f_{1\;k}(r) \\ -ir\; g_{2\;k}(r) \end{pmatrix}. \tag{C26}$$

Then the solution to Eq. (22) is given by

$$\Psi_{j\,m}^{k} = \frac{1}{r}\begin{pmatrix} u_k(r) \\ -i\; v_k(r)(\vec{\sigma}\cdot\vec{n}) \end{pmatrix} \; y_{j\,m}^{k}(\Omega) = \frac{1}{r}\begin{pmatrix} u_k(r)\; y_{j\,m}^{k}(\Omega) \\ i\; v_k(r)\; y_{j\,m}^{-k}(\Omega) \end{pmatrix}. \tag{C27}$$

Throughout the above derivation, use has been made of formulas given in the next Appendix.

In order to see the spin-flavor symmetry in our case, the explicit form of each lowest-order wave function is given as follows in the case of $J^P = 0^-, 1^-$. That these states are degenerate can be easily seen from the eigenvalue equation where the eigenvalue E_0^k depends only on the quantum number k and these states have the same value $k = -1$. Or more explicitly we can show the degeneracy by calculating the wave functions for the two states, $J^P = 0^-, 1^-$. The pseudoscalar state ($J^P = 0^-$) is given by

$$(0 \quad \Psi_{0\,0}^{-1}) = \frac{1}{\sqrt{4\pi}\; r}\begin{pmatrix} 0 & u_{-1}(r) \\ 0 & -i\; v_{-1}(r)\; (\vec{n}\cdot\vec{\sigma}) \end{pmatrix}, \tag{C28}$$

and the vector state ($J^P = 1^-$) is given by

$$\sum_m \; \epsilon^m (0 \quad \Psi_{1\,m}^{-1}) = \frac{i}{\sqrt{4\pi}\; r}\begin{pmatrix} 0 & u_{-1}(r) \\ 0 & -i\; v_{-1}(r)\; (\vec{n}\cdot\vec{\sigma}) \end{pmatrix} \; (\vec{\epsilon}\cdot\vec{\sigma}), \tag{C29}$$

where use has been made of Eqs. (C11) and (C12). These are transformed into each other via the unitary rotation

$$\exp\left(\frac{\pi}{2}\vec{\epsilon}\cdot\vec{\sigma}\right). \tag{C30}$$

Here one has to remember that $\vec{\epsilon}^{\,2}=-1$ and also that we omit the U_c^{-1} operation on the wave function for simplicity. Similar degeneracy can be seen for a pair of states with the same value of k.

APPENDIX D: MATRIX ELEMENTS

In this appendix, we evaluate matrix elements of the RHS of Eqs. (31) and (38) to obtain mass corrections, E_1^k, E_2^k, those of the RHS of Eqs. (32), (39), and (40) to obtain the corrections of Λ_- components of wave functions, $c_{1+}^{\ell k}$, $c_{2+}^{\ell k}$, and to evaluate Eqs. (26) and (36) to obtain the corrections of Λ_+ components of wave functions ψ_i^{ℓ} up to the second order $(i=1,2)$, $c_{1-}^{\ell k}, c_{2-}^{\ell k}$.

Summarizing $\Lambda_- - \Lambda_-$ and/or $\Lambda_- - \Lambda_+$ matrix elements of the Hamiltonian, the following equations are obtained. The RHS of Eq. (26) is given here again as

$$c_{1-}^{\ell k}=\frac{1}{2m_Q}\langle\Psi_k^-|H_0^{-+}|\Psi_\ell^+\rangle = \frac{1}{4m_Q}\langle\Psi_k^-|[\vec{\alpha}_q\cdot\vec{\alpha}_Q+(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})]V|\Psi_\ell^+\rangle, \tag{D1}$$

which requires one to calculate the zeroth order matrix elements. Here one must notice the following relation,

$$c_{1-}^{\ell k}=c_{1-}^{k\ell *}=\frac{1}{2m_Q}\langle\Psi_\ell^+|H_0^{+-}|\Psi_k^-\rangle^\dagger. \tag{D2}$$

The coefficient $c_{1+}^{\ell k}$ is given by, for $\ell\neq k$,

$$c_{1+}^{\ell k}=\frac{1}{E_0^\ell-E_0^k}\left[2m_Q\sum_{\ell'} c_{1-}^{\ell\ell'}c_{1-}^{\ell' k}+\langle\Psi_k^+|H_1^{--}|\Psi_\ell^+\rangle\right]. \tag{D3}$$

Using Eq. (D2), the first-order energy correction is given by

$$E_1^\ell=2m_Q\sum_{\ell'}|c_{1-}^{\ell\ell'}|^2+\langle\Psi_\ell^+|H_1^{--}|\Psi_\ell^+\rangle. \tag{D4}$$

Simplifying Eq. (36), one obtains

$$c_{2-}^{\ell k}=\sum_{\ell'}c_{1+}^{\ell\ell'}c_{1-}^{\ell' k}+\frac{1}{2m_Q}\Bigg[(E_0^k-E_0^\ell)c_{1-}^{\ell k} -2\sum_{\ell'}c_{1-}^{\ell\ell'}\langle\Psi_k^-|\beta_q S|\Psi_{\ell'}^-\rangle+\langle\Psi_k^-|H_1^{-+}|\Psi_\ell^+\rangle\Bigg], \tag{D5}$$

$$c_{2+}^{\ell k}=\frac{1}{E_0^\ell-E_0^k}\Bigg[2m_Q\sum_{\ell'}c_{2-}^{\ell\ell'}c_{1-}^{\ell' k} +\sum_{\ell'}\left(c_{1+}^{\ell\ell'}\langle\Psi_k^+|H_1^{--}|\Psi_{\ell'}^+\rangle +c_{1-}^{\ell\ell'}\langle\Psi_k^+|H_1^{+-}|\Psi_{\ell'}^-\rangle\right)+\langle\Psi_k^+|H_2^{--}|\Psi_\ell^+\rangle -E_1^\ell c_{1+}^{\ell k}\Bigg] \quad \text{for } \ell\neq k, \tag{D6}$$

$$E_2^\ell=2m_Q\sum_{\ell'}c_{2-}^{\ell\ell'}c_{1-}^{\ell'\ell}+\sum_{\ell'}\left(c_{1+}^{\ell\ell'}\langle\Psi_\ell^+|H_1^{--}|\Psi_{\ell'}^+\rangle +c_{1-}^{\ell\ell'}\langle\Psi_\ell^+|H_1^{+-}|\Psi_{\ell'}^-\rangle\right)+\langle\Psi_\ell^+|H_2^{--}|\Psi_\ell^+\rangle. \tag{D7}$$

Although it is apparent that E_1^k is always real from Eq. (D4), it is not clear whether Eq. (D7) is real or not. We will rewrite Eq. (D7) so that reality of E_2^k is manifest as follows.

$$E_2^\ell=\sum_{\ell'}\sum_{\ell''}c_{1-}^{\ell'\ell}\langle\Psi_{\ell'}^-|H_0^{++}|\Psi_{\ell''}^-\rangle c_{1-}^{\ell\ell''}-E_0^\ell\sum_{\ell'}|c_{1-}^{\ell\ell'}|^2 +2\mathrm{Re}\sum_{\ell'}c_{1-}^{\ell'\ell}\langle\Psi_{\ell'}^-|H_1^{-+}|\Psi_\ell^+\rangle +\sum_{\ell'}\frac{1}{E_0^\ell-E_0^{\ell'}}\Bigg(4m_Q^2\Bigg|\sum_{\ell''}c_{1-}^{\ell\ell''}c_{1-}^{\ell''\ell'}\Bigg|^2 +\left|\langle\Psi_\ell^+|H_1^{--}|\Psi_{\ell'}^+\rangle\right|^2 +4m_Q\mathrm{Re}\sum_{\ell''}c_{1-}^{\ell\ell''}c_{1-}^{\ell''\ell'}\langle\Psi_\ell^+|H_1^{--}|\Psi_{\ell'}^+\rangle\Bigg) +\langle\Psi_\ell^+|H_2^{--}|\Psi_\ell^+\rangle, \tag{D8}$$

whose expression is apparently real.

In the above derivation, we have used the projected Hamiltonian at each order, $H_i^{\alpha\beta}$, which is defined by

$$\Lambda_\alpha H_i\Lambda_\beta\equiv\Lambda_\alpha H_i^{\alpha\beta}\Lambda_\beta=\Lambda_\alpha H_i^{\alpha\beta}=H_i^{\alpha\beta}\Lambda_\beta, \tag{D9}$$

where $H_i^{\alpha\beta}$ is composed of Dirac matrices, $\vec{\alpha}$, β, $\vec{\Sigma}$, and γ^5 [13]:

$$H_0^{--}=\vec{\alpha}_q\cdot\vec{p}+\beta_q(m_q+S)+V, \tag{D10a}$$

$$H_0^{-+}=\tfrac{1}{2}[\vec{\alpha}_q\cdot\vec{\alpha}_Q+(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})]V, \tag{D10b}$$

$$H_0^{+-}=H_0^{-+}, \tag{D10c}$$

$$H_0^{++}=\vec{\alpha}_q\cdot\vec{p}+\beta_q(m_q-S)+V, \tag{D10d}$$

$$H_1^{--}=\frac{1}{2m_Q}\Bigg\{\vec{p}^{\,2}+V[(\vec{\alpha}_q\cdot\vec{p})-i(\vec{\alpha}_q\cdot\vec{n})\partial_r]-V'\Bigg[i(\vec{\alpha}_q\cdot\vec{n}) +\frac{1}{2}(\vec{\alpha}_q\cdot\vec{\Sigma}_Q\times\vec{n})\Bigg]-\frac{1}{r}V\Bigg[i(\vec{\alpha}_q\cdot\vec{n}) -\frac{1}{2}(\vec{\alpha}_q\cdot\vec{\Sigma}_Q\times\vec{n})\Bigg]\Bigg\}, \tag{D10e}$$

$$H_1^{-+}=\frac{1}{m_Q}\left[-S\beta_q\ (\vec{\alpha}_Q\cdot\vec{p})+\frac{i}{2}(\beta_q\ S'+V')(\vec{\alpha}_Q\cdot\vec{n})\right], \tag{D10f}$$

$$H_1^{+-}=\frac{1}{m_Q}\left[-S\beta_q\ (\vec{\alpha}_Q\cdot\vec{p})+\frac{i}{2}(\beta_q\ S'-V')(\vec{\alpha}_Q\cdot\vec{n})\right], \tag{D10g}$$

$$H_1^{++}=-H_1^{--}, \tag{D10h}$$

$$H_2^{--}=\frac{1}{2m_Q^2}\left\{-\beta_q\left(\vec{p}+\frac{1}{2}\vec{q}\right)^2 S+\frac{1}{4}\Delta V+\frac{1}{2r}(\beta_q\ S'-V')\ (\vec{\Sigma}_Q\cdot\vec{\ell})\right\}, \tag{D10i}$$

$$H_2^{-+}=-\frac{1}{8m_Q^2}\left\{2V[(\vec{\alpha}_q\cdot\vec{p})-i\ (\vec{\alpha}_q\cdot\vec{n})\partial_r](\vec{\alpha}_Q\cdot\vec{p})-2iV'(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{p})-iV'(\vec{\alpha}_Q\cdot\vec{n})[(\vec{\alpha}_q\cdot\vec{p})-i\ (\vec{\alpha}_q\cdot\vec{n})\partial_r]+\frac{1}{r}V'(\vec{\alpha}_q\cdot\vec{\ell})\gamma_Q^5\right\}$$
$$+\frac{1}{8m_Q^2 r}V\left\{3i\ (\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{p})+[(\vec{\alpha}_q\cdot\vec{\alpha}_Q)-2(\vec{\alpha}_q\cdot\vec{n})(\vec{\alpha}_Q\cdot\vec{n})]\partial_r+\frac{1}{r}(\vec{\alpha}_q\cdot\vec{\ell})\ \gamma_Q^5\right\}, \tag{D10j}$$

$$H_2^{+-}=H_2^{-+}, \tag{D10k}$$

$$H_2^{++}=\frac{1}{2m_Q^2}\left\{\beta_q\left(\vec{p}+\frac{1}{2}\vec{q}\right)^2 S+\frac{1}{4}\Delta V-\frac{1}{2r}(\beta_q\ S'+V')\ (\vec{\Sigma}_Q\cdot\vec{\ell})\right\}. \tag{D10l}$$

Use has been made of the following formulas for the gamma matrices,

$$\beta_Q\Lambda_\pm=\pm\Lambda_\pm,\quad \vec{\alpha}_Q\Lambda_\pm=\Lambda_\mp\vec{\alpha}_Q,\quad \vec{\Sigma}_Q\Lambda_\pm=\Lambda_\pm\vec{\Sigma}_Q,$$
$$\vec{\gamma}_Q\Lambda_\pm=\Lambda_\mp\vec{\gamma}_Q=\mp\vec{\alpha}_Q\Lambda_\pm,$$
$$\beta_Q\vec{\Sigma}_Q\Lambda_\pm=\pm\Lambda_\pm\vec{\Sigma}_Q,\quad \gamma_Q^5\Lambda_\pm=\Lambda_\mp\gamma_Q^5. \tag{D11}$$

Matrix elements of interaction terms among eigenfunctions are calculated below. Degeneracy can be resolved by heavy quark spin-dependent terms which includes $\vec{\alpha}_Q$ and/or $\vec{\Sigma}_Q$ dependent terms, i.e., the last terms of H_1^{--} and H_2^{--} together with contributions from negative components of the wave functions coming from H_0^{-+} and H_1^{-+}.

The formulas necessary for calculating the matrix elements are given below when operators, $(\vec{\sigma}_q\cdot\vec{n})$, $(\vec{\sigma}_q\cdot\vec{\ell})$, $(\vec{\sigma}_q\cdot\vec{p})$, $(\vec{\sigma}_Q\cdot\vec{\ell})$, $\vec{\sigma}_q\cdot(\vec{\sigma}_Q\times\vec{n})$, $(\vec{\sigma}_q\cdot\vec{\sigma}_Q)$, $(\vec{\sigma}_Q\cdot\vec{n})$, and $(\vec{\sigma}_Q\cdot\vec{p})$, operate on the function, $y_{j\,m}^k(\Omega)$ or $f(r)\ y_{j\,m}^k(\Omega)$. The symbol, $\otimes$, is used in the same meaning for 4×4 gamma matrices, i.e., Pauli matrices for a light anti-quark are multiplied from left while those for a heavy quark from right:

$$(\vec{\sigma}_q\cdot\vec{n})\otimes\ y_{j\,m}^k=-y_{j\,m}^{-k}, \tag{D12}$$

$$(\vec{\sigma}_q\cdot\vec{\ell})\otimes\ y_{j\,m}^k=-(k+1)\ y_{j\,m}^k, \tag{D13}$$

$$(\vec{\sigma}_q\cdot\vec{p})\otimes\ f(r)\ y_{j\,m}^k=i\left(\partial_r+\frac{k+1}{r}\right)f(r)\ y_{j\,m}^{-k}=-i\left(\partial_r+\frac{k+1}{r}\right)f(r)\ (\vec{\sigma}_q\cdot\vec{n})\otimes\ y_{j\,m}^k, \tag{D14}$$

$$(\vec{\sigma}_Q\cdot\vec{\ell})\otimes\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}=\frac{1}{2j+1}\begin{pmatrix}j(2j+3) & 2\sqrt{j(j+1)}\\ 2\sqrt{j(j+1)} & -(2j-1)(j+1)\end{pmatrix}\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}, \tag{D15}$$

$$(\vec{\sigma}_Q\cdot\vec{\ell})\otimes\begin{pmatrix}y_{j\,m}^{j+1}\\ y_{j\,m}^{-j}\end{pmatrix}=\begin{pmatrix}j+2 & 0\\ 0 & -(j-1)\end{pmatrix}\begin{pmatrix}y_{j\,m}^{j+1}\\ y_{j\,m}^{-j}\end{pmatrix},$$

$$(\vec{\sigma}_q\cdot\vec{\sigma}_Q\times\vec{n})\otimes\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}=\frac{2i}{2j+1}\begin{pmatrix}-(j+1) & \sqrt{j(j+1)}\\ \sqrt{j(j+1)} & -j\end{pmatrix}\begin{pmatrix}y_{j\,m}^{j+1}\\ y_{j\,m}^{-j}\end{pmatrix}, \tag{D16}$$

$$(\vec{\sigma}_q\cdot\vec{\sigma}_Q\times\vec{n})\otimes\begin{pmatrix}y_{j\,m}^{j+1}\\ y_{j\,m}^{-j}\end{pmatrix}=\frac{-2i}{2j+1}\begin{pmatrix}-(j+1) & \sqrt{j(j+1)}\\ \sqrt{j(j+1)} & -j\end{pmatrix}\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}.$$

$$(\vec{\sigma}_q\cdot\vec{\sigma}_Q)\otimes\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}=\frac{1}{2j+1}\begin{pmatrix}2j+3 & -4\sqrt{j(j+1)}\\ -4\sqrt{j(j+1)} & 2j-1\end{pmatrix}\begin{pmatrix}y_{j\,m}^{-(j+1)}\\ y_{j\,m}^{j}\end{pmatrix}, \tag{D17}$$

$$(\vec{\sigma}_q\cdot\vec{\sigma}_Q)\otimes\begin{pmatrix} y_{j\,m}^{j+1} \\ y_{j\,m}^{-j}\end{pmatrix} = -\begin{pmatrix} y_{j\,m}^{j+1} \\ y_{j\,m}^{-j}\end{pmatrix},$$

$$(\vec{\sigma}_Q\cdot\vec{n})\otimes\begin{pmatrix} y_{j\,m}^{-(j+1)} \\ y_{j\,m}^{j}\end{pmatrix} = \frac{-1}{2j+1}\begin{pmatrix} 1 & -2\sqrt{j(j+1)} \\ -2\sqrt{j(j+1)} & -1\end{pmatrix}\begin{pmatrix} y_{j\,m}^{-(j+1)} \\ y_{j\,m}^{j}\end{pmatrix}, \tag{D18}$$

$$(\vec{\sigma}_Q\cdot\vec{n})\otimes\begin{pmatrix} y_{j\,m}^{j+1} \\ y_{j\,m}^{-j}\end{pmatrix} = \frac{-1}{2j+1}\begin{pmatrix} 1 & -2\sqrt{j(j+1)} \\ -2\sqrt{j(j+1)} & -1\end{pmatrix}\begin{pmatrix} y_{j\,m}^{j+1} \\ y_{j\,m}^{-j}\end{pmatrix},$$

$$(\vec{\sigma}_Q\cdot\vec{p})\otimes\begin{pmatrix} f(r)\,y_{j\,m}^{-(j+1)} \\ f(r)\,y_{j\,m}^{j}\end{pmatrix} = \frac{i}{2j+1}\begin{pmatrix} \partial_r-\dfrac{j}{r} & -2\sqrt{j(j+1)}\left(\partial_r+\dfrac{j+1}{r}\right) \\ -2\sqrt{j(j+1)}\left(\partial_r-\dfrac{j}{r}\right) & -\left(\partial_r+\dfrac{j+1}{r}\right)\end{pmatrix}\begin{pmatrix} f(r)\,y_{j\,m}^{-(j+1)} \\ f(r)\,y_{j\,m}^{j}\end{pmatrix}, \tag{D19}$$

$$(\vec{\sigma}_Q\cdot\vec{p})\otimes\begin{pmatrix} f(r)\,y_{j\,m}^{j+1} \\ f(r)\,y_{j\,m}^{-j}\end{pmatrix} = \frac{i}{2j+1}\begin{pmatrix} \partial_r+\dfrac{j+2}{r} & -2\sqrt{j(j+1)}\left(\partial_r+\dfrac{j+2}{r}\right) \\ -2\sqrt{j(j+1)}\left(\partial_r-\dfrac{j-1}{r}\right) & -\left(\partial_r-\dfrac{j-1}{r}\right)\end{pmatrix}\begin{pmatrix} f(r)\,y_{j\,m}^{j+1} \\ f(r)\,y_{j\,m}^{-j}\end{pmatrix},$$

1. $\Lambda_- - \Lambda_-$ matrix elements

a. First-order terms

To calculate Eqs. (31) and (32), one needs the following $\Lambda_- - \Lambda_-$ matrix elements,

$$\langle\Psi^+_{\ell'}|H_1^{--}|\Psi^+_{\ell}\rangle = \left\langle \Psi^+_{\ell'}\left|\frac{1}{2m_Q}\{\vec{p}^2+V[(\vec{\alpha}_q\cdot\vec{p})-i\,(\vec{\alpha}_q\cdot\vec{n})\partial_r]-V'(\vec{\alpha}_q\cdot\vec{\Sigma}_Q\times\vec{n})\}\right|\Psi^+_{\ell}\right\rangle$$
$$=\frac{1}{2}\mathrm{tr}\int d^3r\Psi_{j\,m}^{k'\,\dagger}\frac{1}{2m_Q}\{\vec{p}^2+V[(\vec{\alpha}_q\cdot\vec{p})-i\,(\vec{\alpha}_q\cdot\vec{n})\partial_r]-V'(\vec{\alpha}_q\cdot\vec{\sigma}_Q\times\vec{n})\}\otimes\Psi_{j\,m}^{k}, \tag{D20}$$

where the sets of quantum numbers are given by $\ell=(j,\,m,\,k)$ and $\ell'=(j,\,m,\,k')$. Some simplification occurs because $V(r)\sim 1/r$ hence $V'=-V/r$. Each matrix element of the first-order interaction terms is given below.

$$\frac{1}{2}\mathrm{tr}\int d^3r\Psi_{j\,m}^{k\,\dagger}\vec{p}^{\,2}\otimes\Psi_{j\,m}^{k} = \frac{1}{2}\mathrm{tr}\int d^3r\Psi_{j\,m}^{k\,\dagger}(\vec{\Sigma}_q\cdot\vec{p})^2\otimes\Psi_{j\,m}^{k} = \int dr\Phi_k^\dagger\begin{pmatrix} -\partial_r^2+\dfrac{k(k+1)}{r^2} & 0 \\ 0 & -\partial_r^2+\dfrac{k(k-1)}{r^2}\end{pmatrix}\Phi_k, \tag{D21}$$

$$\frac{1}{2}\mathrm{tr}\int d^3r\Psi_{j\,m}^{k\,\dagger}V[(\vec{\alpha}_q\cdot\vec{p})-i\,(\vec{\alpha}_q\cdot\vec{n})\partial_r]\otimes\Psi_{j\,m}^{k} = \int dr\Phi_k^\dagger\begin{pmatrix} 0 & -V\left(2\partial_r-\dfrac{k+1}{r}\right) \\ V\left(2\partial_r+\dfrac{k-1}{r}\right) & 0\end{pmatrix}\Phi_k, \tag{D22}$$

where $\Phi_k(r)$ is defined by Eq. (C26) in the Appendix C. Some nonvanishing matrix elements of the last term of Eq. (D20) are given by

$$\langle \Psi_{\ell'}^{+} | V' (\vec{\alpha}_q \cdot \vec{\Sigma}_Q \times \vec{n}) \, | \Psi_{\ell}^{+} \rangle = \begin{cases} \dfrac{-2k}{2k+1} \displaystyle\int dr \Phi_k^{\dagger} V' \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_k & \text{for } k = -(j+1),\ j, \\ \dfrac{2k}{2k-1} \displaystyle\int dr \Phi_k^{\dagger} V' \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_k & \text{for } k = j+1, -j, \\ \dfrac{2\sqrt{j(j+1)}}{2j+1} \displaystyle\int dr \Phi_j^{\dagger} V' \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_{-(j+1)}, & \\ -\dfrac{2\sqrt{j(j+1)}}{2j+1} \displaystyle\int dr \Phi_{-j}^{\dagger} V' \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_{j+1}, & \end{cases} \tag{D23}$$

and their complex conjugates.

b. Second-order terms

To calculate Eqs. (38) and (39), one needs the following $\Lambda_- - \Lambda_-$ matrix elements,

$$\begin{aligned} \langle \Psi_{\ell'}^{+} | H_2^{--} | \Psi_{\ell}^{+} \rangle &= \left\langle \Psi_{\ell'}^{+} \left| \frac{1}{2m_Q^2} \left\{ -\beta_q \left(\vec{p} + \frac{1}{2}\vec{q} \right)^2 S + \frac{1}{4} \Delta V + \frac{1}{2r} (\beta_q S' - V') \, (\vec{\alpha}_Q \cdot \vec{\ell}) \right\} \right| \Psi_{\ell}^{+} \right\rangle, \\ &= \frac{1}{2} \mathrm{tr} \int d^3 r \Psi_{j\ m}^{k'\ \dagger} \frac{1}{2m_Q^2} \left\{ -\beta_q \left(\vec{p} + \frac{1}{2}\vec{q} \right)^2 S + \frac{1}{4} \Delta V + \frac{1}{2r} (\beta_q S' - V') \, (\vec{\sigma}_Q \cdot \vec{\ell}) \right\} \otimes \Psi_{j\ m}^{k}. \end{aligned} \tag{D24}$$

Each matrix element of the second-order interaction terms is given below.

$$\frac{1}{2} \mathrm{tr} \int d^3 r \Psi_{j\ m}^{k\ \dagger} \beta_q \left(\vec{p} + \frac{1}{2}\vec{q} \right)^2 S \otimes \Psi_{j\ m}^{k} = \int dr \Phi_k^{\dagger} \begin{pmatrix} S_+ & 0 \\ 0 & -S_- \end{pmatrix} \Phi_k, \tag{D25}$$

where

$$S_{\pm} = S \left[-\partial_r^2 + \frac{k(k \pm 1)}{r^2} \right] - S' \left(\partial_r - \frac{1}{2r} \right). \tag{D26}$$

Since $V = -4\alpha_s/3r$ and $\Delta\, 1/r = -4\pi\delta^3(\vec{r})$, we need to calculate

$$\frac{1}{2} \mathrm{tr} \int d^3 r \Psi_{j\ m}^{k'\ \dagger} \Delta \frac{1}{r} \otimes \Psi_{j\ m}^{k} = -|\Phi_k(0)|^2 \ \delta_{k,\ k'}. \tag{D27}$$

Nonvanishing matrix elements of the last term of Eq. (D24) are given by

$$\left\langle \Psi_{\ell'}^{+} \left| \frac{1}{r} (\beta_q S' - V') \, (\vec{\alpha}_Q \cdot \vec{\ell}) \right| \Psi_{\ell}^{+} \right\rangle$$

$$= \begin{cases} \displaystyle\int dr \ \ \Phi_k^{\dagger} \begin{pmatrix} -\dfrac{(k+1)(2k-1)}{2k+1} \left(\dfrac{S'}{r} - \dfrac{V'}{r} \right) & 0 \\ 0 & (k-1) \left(\dfrac{S'}{r} + \dfrac{V'}{r} \right) \end{pmatrix} \Phi_k & \text{for } k = -(j+1),\ j, \\ \displaystyle\int dr \ \ \Phi_k^{\dagger} \begin{pmatrix} (k+1) \left(\dfrac{S'}{r} - \dfrac{V'}{r} \right) & 0 \\ 0 & -\dfrac{(k-1)(2k+1)}{2k-1} \left(\dfrac{S'}{r} + \dfrac{V'}{r} \right) \end{pmatrix} \Phi_k & \text{for } k = j+1, -j, \\ \dfrac{2\sqrt{j(j+1)}}{2j+1} \displaystyle\int dr \Phi_j^{\dagger} \left(\dfrac{S'}{r} - \dfrac{V'}{r} \right) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \Phi_{-(j+1)}, & \\ -\dfrac{2\sqrt{j(j+1)}}{2j+1} \displaystyle\int dr \Phi_{-j}^{\dagger} \left(\dfrac{S'}{r} + \dfrac{V'}{r} \right) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Phi_{j+1}, & \end{cases} \tag{D28}$$

and their complex conjugates.

2. $\Lambda_- - \Lambda_+$ matrix elements

a. Zeroth-order terms

Among the many $\Lambda_- - \Lambda_+$ components, that of the RHS of Eq. (26) is the only matrix element to be needed in the later calculations at the zeroth order, which is again given here:

$$\langle \Psi^-_{\ell'} | H_0^{-+} | \Psi^+_{\ell} \rangle = \left\langle \Psi^-_{\ell'} \left| \frac{1}{2}[\ \vec{\alpha}_q \cdot \vec{\alpha}_Q + (\vec{\alpha}_q \cdot \vec{n})(\vec{\alpha}_Q \cdot \vec{n})\ ] V \right| \Psi^+_{\ell} \right\rangle,$$
$$= \frac{1}{2}\mathrm{tr} \int d^3 r \Psi^{k'\dagger}_{j\,m} \frac{1}{2}[\ \vec{\alpha}_q \cdot \vec{\sigma}_Q + (\vec{\alpha}_q \cdot \vec{n})(\vec{\sigma}_Q \cdot \vec{n})\ ] V \otimes \Psi^k_{j\,m}. \tag{D29}$$

Nonvanishing matrix elements are given by

$$\langle \Psi^-_{\ell'} | (\vec{\alpha}_q \cdot \vec{\alpha}_Q)\ V | \Psi^+_{\ell} \rangle = \begin{cases} \int dr\ \Phi^\dagger_{-k} \begin{pmatrix} 0 & -1 \\ \frac{2k-1}{2k+1} & 0 \end{pmatrix} V\Phi_k \quad \text{for } k = -(j+1),\ \ j, \\ -\frac{4\sqrt{j(j+1)}}{2j+1} \int dr\ \Phi^\dagger_{-j} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} V\Phi_{-(j+1)}, \\ -\frac{4\sqrt{j(j+1)}}{2j+1} \int dr\ \Phi^\dagger_{j} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} V\Phi_{j+1}, \end{cases} \tag{D30}$$

and

$$\langle \Psi^-_{\ell'} | (\vec{\alpha}_q \cdot \vec{n})(\vec{\alpha}_Q \cdot \vec{n}) V | \Psi^+_{\ell} \rangle = \begin{cases} \frac{i}{2k+1} \int dr\ \Phi^\dagger_{-k} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} V\Phi_k \quad \text{for } k = -(j+1),\ \ j, \\ \frac{2i\sqrt{j(j+1)}}{2j+1} \int dr\ \Phi^\dagger_{-j} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} V\Phi_{-(j+1)}, \end{cases} \tag{D31}$$

and their complex conjugates.

b. First-order terms

The first order $\Lambda_- - \Lambda_+$ matrix element is given by

$$\langle \Psi^-_{\ell'} | H_1^{-+} | \Psi^+_{\ell} \rangle = \left\langle \Psi^-_{\ell'} \left| \frac{1}{m_Q}\left[-S\beta_q\ (\vec{\alpha}_Q \cdot \vec{p}) + \frac{i}{2}(\beta_q\ S' + V')(\vec{\alpha}_Q \cdot \vec{n}) \right] \right| \Psi^+_{\ell} \right\rangle,$$
$$= \frac{1}{2}\mathrm{tr} \int d^3 r \Psi^{k'\dagger}_{j\,m} \frac{1}{m_Q}\left[-S\beta_q\ (\vec{\sigma}_Q \cdot \vec{p}) + \frac{i}{2}(\beta_q\ S' + V')(\vec{\sigma}_Q \cdot \vec{n}) \right] \otimes \Psi^k_{j\,m}. \tag{D32}$$

Nonvanishing matrix elements are given by, for $k = -(j+1)$, or j,

$$\langle \Psi^-_{\ell'} | S\beta_q\ (\vec{\alpha}_Q \cdot \vec{p}) | \Psi^+_{\ell} \rangle = \begin{cases} \frac{-i}{2k+1} \int dr\ \Phi^\dagger_{-k} S \begin{pmatrix} \partial_r + \frac{k+1}{r} & 0 \\ 0 & -\partial_r + \frac{k-1}{r} \end{pmatrix} \Phi_k, \\ \frac{-2i\sqrt{j(j+1)}}{2j+1} \int dr\ \Phi^\dagger_{k+1} S \begin{pmatrix} \partial_r - \frac{k}{r} & 0 \\ 0 & -\partial_r + \frac{k-1}{r} \end{pmatrix} \Phi_k, \end{cases} \tag{D33}$$

and

$$\langle \Psi_{\ell'}^{-}|(\beta_q S'+V')(\vec{\alpha}_Q\cdot\vec{n})|\Psi_{\ell}^{+}\rangle = \begin{cases} \dfrac{1}{2k+1}\displaystyle\int dr\ \Phi_k^{\dagger}\begin{pmatrix} S'+V' & 0 \\ 0 & -S'+V' \end{pmatrix}\Phi_k, \\ \dfrac{2\sqrt{j(j+1)}}{2j+1}\displaystyle\int dr\ \Phi_j^{\dagger}\begin{pmatrix} S'+V' & 0 \\ 0 & -S'+V' \end{pmatrix}\Phi_{-(j+1)}, \end{cases} \tag{D34}$$

and their complex conjugates. Note that when one takes complex conjugate, derivative operators do not operate on S' and V', but on a wave function, Φ_{ℓ}.

Calculating all the matrix elements of the Hamiltonian given in Sec. II or Appendix D, the results are summarized in the following two matrices. Matrix elements of the Hamiltonian among $\langle\Psi_{\ell}^{+}|$ and $|\Psi_{\ell'}^{+}\rangle$, or those of the interaction terms, m_Q, H_0^{--}, H_1^{--}, and H_2^{--}, among eigenfunctions $\Psi_{j\ m}^{k\ \dagger}$ and $\Psi_{j\ m}^{k'}$ obtained above are given by, up to the second order in $1/m_Q$,

$$\begin{pmatrix} U_{-1,0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & U_{-1,1} & 0 & 0 & 0 & 0 & V^1_{-1,2} & 0 \\ 0 & 0 & U_{1,0} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U_{1,1} & V^1_{1,-2} & 0 & 0 & 0 \\ 0 & 0 & 0 & V^1_{-2,1} & U_{-2,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & U_{-2,2} & 0 & 0 \\ 0 & V^1_{2,-1} & 0 & 0 & 0 & 0 & U_{2,1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & U_{2,2} \end{pmatrix}, \tag{D35}$$

where

$$U_{k,\ j}=m_Q+E_0^k+U_{k,\ j}^{(1)}+U_{k,\ j}^{(2)},\quad V_{k,\ k'}^{j}=V_{k,\ k'}^{(1)\ j}+V_{k,\ k'}^{(2)\ j},$$

$$\langle\Psi_{\ell}^{+}|H_i|\Psi_{\ell'}^{+}\rangle=\frac{1}{2}\mathrm{tr}\int d^3r\Psi_{j\ m}^{k\ \dagger}H_i^{--}\otimes\Psi_{jm}^{k'}=U_{k,\ j}^{(i)}\ \delta_{k\ k'}+V_{k,k'}^{(i)\ j}\quad \text{for}\ \ i=1,2. \tag{D36}$$

Here the matrix elements are written in the k and j space and subscripts i for E_i^k and superscripts i for $U_{k,j}^{(i)}$ and $V_{k,k'}^{(i)\ j}$ mean the ith order in $1/m_Q$, k and k' for E_i^k, $U_{k,j}^{(i)}$, and $V_{k,k'}^{(i)\ j}$ stand for k quantum number, and j for the total angular momentum. For instance, $V_{k,k'}^{(2)\ j}$ means the matrix element of the third term of H_2^{--} between $\Psi_{jm}^{k\ \dagger}$ and $\Psi_{jm}^{k'}$ given by 1/2 of Eq. (D24), i.e.,

$$V_{j,\ -(j+1)}^{(2)}=\frac{\sqrt{j(j+1)}}{2j+1}\int dr\Phi_j^{\dagger}\left(\frac{S'}{r}-\frac{V'}{r}\right)\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}\Phi_{-(j+1)}.$$

As for the $\Lambda_- - \Lambda_+$ matrix elements of the Hamiltonian, we only need nonvanishing matrix elements of H_0^{-+} or $c_{1-}^{\ell\ k}$ as one can see from Eqs. (D1)–(D8) up to the second order in $1/m_Q$, which are given below.

$$\begin{pmatrix} 0 & 0 & c_{1-}^{-1,1}(0) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{1-}^{-1,1}(1) & c_{1-}^{-1,-2}(1) & 0 & 0 & 0 \\ c_{1-}^{1,-1}(0) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_{1-}^{1,-1}(1) & 0 & 0 & 0 & 0 & c_{1-}^{1,2}(1) & 0 \\ 0 & c_{1-}^{-2,-1}(1) & 0 & 0 & 0 & 0 & c_{1-}^{-2,2}(1) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & c_{1-}^{-2,2}(2) \\ 0 & 0 & 0 & c_{1-}^{2,1}(1) & c_{1-}^{2,-2}(1) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{1-}^{2,-2}(2) & 0 & 0 \end{pmatrix}, \tag{D37}$$

where the integer in the brackets is a value of a total angular momentum, j, and it turns out that this matrix is Hermitian, i.e., $c_{1-}^{\ell\ k}(j_0)=c_{1-}^{k\ \ell}(j_0)^*$ for the same value of $j=j_0$. The $\Lambda_+ - \Lambda_-$ matrix elements are the complex conjugate of the above matrix, Eq. (D37).

With these matrix elements, the total energy, E^{ℓ}, is calculated by Eqs. (D4) and (D8) together with m_Q and an eigenvalue, E_0^k, of Eq. (C25) up to the second order in $1/m_Q$. Degeneracy between the states with the same value of k in the leading order can be resolved by diagonal as well as off-diagonal matrix elements of the last terms of H_1^{--} and H_2^{--} together with contributions from negative components of the wave functions coming from H_0^{-+} and H_1^{-+} as mentioned earlier.

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