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On enhanced corrections from quasi-degenerate states to heavy quarkonium observables

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ABSTRACT

It is well known that in perturbation theory existence of quasi-degenerate states can rearrange the order counting. For a heavy quarkonium system, naively, enhanced effects (l-changing mixing effects) could contribute already to the first-order and third-order corrections to the wave function and the energy level, respectively, in expansion in α_s. We present a formulation and note that the corresponding (lowest-order) corrections vanish due to absence of the relevant off-diagonal matrix elements. As a result, in the quarkonium energy level and leptonic decay width, the enhanced effects are expected to appear, respectively, in the fifth- and fourth-order corrections and beyond.

1. Introduction

Heavy quarkonium, the bound state of a heavy quark–antiquark pair, is a prime example of a strongly interacting system whose properties are well documented in perturbative QCD. With the advent of new theoretical framework, such as effective field theory (EFT) and threshold expansion technique, as well as proper treatment for decoupling infrared degrees of freedom, the heavy quarkonium system has become an ideal laboratory for precision tests of predictions of perturbative QCD with respect to various experimental data and lattice QCD predictions.

The state-of-the-art computational results in this field comprise the next-to-next-to-next-to-leading order (NNNLO) energy levels of heavy quarkonium [1–3], the NNNLO pair-production cross section of heavy quarks near threshold [4,5], and the leptonic decay width of $\Upsilon(1S)$ state [6]. These calculations utilize the modern EFT, potential-nonrelativistic QCD (pNRQCD) [7,8], for systematically organizing the perturbative expansions in α_s and v (velocity of heavy quarks) in a sophisticated manner. This EFT describes interactions of a non-relativistic quantum mechanical system (dictated by the Schrödinger equation) with ultrasoft gluons, which is organized in multipole expansion. We can benefit from methods and knowledge of perturbation theory of quantum mechanics therein.

It is widely known that quasi-degenerate systems need special care in perturbation theory of quantum mechanics [9], however, thus far the relevant consideration seems to be missing in the computation of the aforementioned NNNLO heavy quarkonium observables.[1] In perturbative expansion of the heavy quarkonium system, the leading-order Hamiltonian is that of the Coulomb system whose energy eigenvalues are labeled only by the principal quantum number n. The first-order correction resolves the degeneracy in the orbital angular momentum l, while the second-order correction resolves the degeneracy in the total spin s and total angular momentum j. Once these features are properly taken into account in perturbative calculations there are enhanced contributions which rearrange the order counting. These are the mixing effects between different l states for the same n. One finds that naively these start from the third-order corrections to the heavy quarkonium energy levels and from the first-order corrections to the wave functions.[2] The latter would induce second-order

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[1] In the computation of the NNLO energy levels the corrections from quasi-degenerate states for the $n \le 3$ states were explicitly considered and found to be absent [10].

[2] As a simple example, consider a matrix

$$\begin{pmatrix} 0 & x^2 V_2 \\ x^2 V_2^* & x V_1 \end{pmatrix}.$$

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corrections to the heavy quark threshold production cross section (or the quarkonium leptonic decay width). By explicit computation the relevant lowest order off-diagonal matrix elements for these corrections vanish. Hence, these enhanced corrections are pushed to higher orders. We present a necessary formulation, an explicit computation at the lowest order, and discuss further higher-order effects.

It is not our purpose to claim originality of the present work but rather to recollect relevant information and to clarify the basis for systematic computation. A closely related subject is the inclusion of transitions (mixings) between two quasi-degenerate states given by off-diagonal matrix elements of interaction operators considered in many potential-model calculations [11–14]. However, (somewhat to our surprise) systematic order counting in light of pNRQCD in expansion in α_s and v has not been addressed so far.

In the case of QED, it was already pointed out in the late 1940s and 1950s that contributions from quasi-degenerate states to the positronium energy levels do not appear at and below order α^6 (order α^4 relative to the LO energy levels); see Ref. [15] and references therein. However, the situations of positronium and heavy quarkonium systems differ in some aspects and it is worth clarifying the latter case explicitly. The crucial difference stems from the fact that the degeneracy of the heavy quarkonium energy level is lifted at α_s^3 whereas the degeneracy is lifted at α^4 in the case of positronium.

2. Perturbation theory for quasi-degenerate system

Consider the Schrödinger equation of heavy quarkonium

$$\left(H^{(0)}+\sum_{i=1}^{\infty}\varepsilon^i V^{(i)}\right)|\Psi_{nlsj}\rangle = E_{nlsj}\,|\Psi_{nlsj}\rangle\,, \tag{1}$$

which dictates the quantum mechanical subsystem in pNRQCD. An expansion parameter ε (corresponding to α_s or v) is introduced,[3] and a unique order in ε is assigned to each potential operator $V^{(i)}$. The definitions of $H^{(0)}, V^{(1)}, \ldots$ can be found, for instance, in [16,3], but we do not need their explicit forms in this section. The energy level and the wave function are labeled with (n,l,s,j). The operators $H^{(0)}$ and $V^{(1)}$ preserve l, s and j. Furthermore, $H^{(0)}$ and $V^{(i)}$ preserve s and j (see Sec. 4), hence we suppress these two labels in the following. ($|nl\rangle = |nlsj\rangle$ represents an eigenstate of $H^{(0)}$.)

The perturbative expansion of the energy level is given by

$$\begin{aligned}
E_{nlsj} &= E_n^{(0)} + \varepsilon E_{nl}^{(1)} + \varepsilon^2\left[\langle nl|\,V^{(2)}\,|nl\rangle + \sum_{n'\neq n}\frac{|\,\langle nl|\,V^{(1)}\,|n'l\rangle\,|^2}{E_n^{(0)}-E_{n'}^{(0)}}\right] \\
&\quad + \varepsilon^3\Bigg[\langle nl|\,V^{(3)}\,|nl\rangle + \sum_{l'\neq l}\frac{|\,\langle nl|\,V^{(2)}\,|nl'\rangle\,|^2}{E_{nl}^{(1)}-E_{nl'}^{(1)}} + \sum_{n'\neq n}\frac{\langle nl|\,V^{(2)}\,|n'l\rangle\,\langle n'l|\,V^{(1)}\,|nl\rangle}{E_n^{(0)}-E_{n'}^{(0)}} \\
&\quad + \sum_{n'\neq n}\frac{\langle nl|\,V^{(1)}\,|n'l\rangle}{E_n^{(0)}-E_{n'}^{(0)}}\left\{\langle n'l|\,V^{(2)}\,|nl\rangle - E_{nl}^{(1)}\frac{\langle n'l|\,V^{(1)}\,|nl\rangle}{E_n^{(0)}-E_{n''}^{(0)}} + \sum_{n''\neq n}\frac{\langle n'l|\,V^{(1)}\,|n''l\rangle\,\langle n''l|\,V^{(1)}\,|nl\rangle}{E_n^{(0)}-E_{n''}^{(0)}}\right\}\Bigg] + \mathcal{O}(\varepsilon^4),
\end{aligned} \tag{2}$$

where we use short-hand notations $E_n^{(0)} \equiv \langle nl|\,H^{(0)}\,|nl\rangle$, $E_{nl}^{(1)} \equiv \langle nl|\,V^{(1)}\,|nl\rangle$. The fourth- and fifth-order corrections will be given in eqs. (16), (17). The subscript of $E_n^{(0)}$ indicates that the leading energy eigenvalue depends only on n, and that of $E_{nl}^{(1)}$ indicates that degeneracy in l is resolved at the first-order. The degeneracy is fully resolved at the second order.

The ε^3-term proportional to $|\,\langle nl|\,V^{(2)}\,|nl'\rangle\,|^2$ in eq. (2) is the main focus of this letter. This correction has not been considered explicitly in the previous studies [1–3]. Since the operator $V^{(2)}$ is accompanied by ε^2, naive order counting indicates that the $|\,\langle nl|\,V^{(2)}\,|nl'\rangle\,|^2$ term may be order ε^4. Due to the quasi-degeneracy of the states $|nl\rangle$ and $|nl'\rangle$, however, the denominator $(E_{nl}^{(1)}-E_{nl'}^{(1)})$ compensates one ε, rendering the term to be order ε^3.

The perturbative expansion of the wave function is given by

$$|\Psi_{nlsj}\rangle = |nlsj\rangle + \sum_{i=1}^{\infty}\varepsilon^i\left[\sum_{l'\neq l}|nl'sj\rangle\,\frac{c_{nl';nl}^{(i)}}{E_{nl}^{(1)}-E_{nl'}^{(1)}} + \sum_{n'\neq n,\ l'}|n'l'sj\rangle\,\frac{d_{n'l';nl}^{(i)}}{E_n^{(0)}-E_{n'}^{(0)}}\right], \tag{3}$$

where $|\Psi_{nlsj}\rangle$ is normalized as $\langle nlsj|\Psi_{nlsj}\rangle = 1$. The coefficients are given by

$$c_{nl';nl}^{(1)} = \langle nl'|\,V^{(2)}\,|nl\rangle\,, \qquad d_{n'l';nl}^{(1)} = \langle n'l'|\,V^{(1)}\,|nl\rangle\,, \tag{4}$$

$$c_{nl';nl}^{(2)} = \langle nl'|\,V^{(3)}\,|nl\rangle + \langle nl'|\,V^{(2)}\,|nl'\rangle\,\frac{c_{nl';nl}^{(1)}}{E_{nl}^{(1)}-E_{nl'}^{(1)}} + \sum_{i=1}^{2}\sum_{n''\neq n,\ l''}\langle nl'|\,V^{(3-i)}\,|n''l''\rangle\,\frac{d_{n''l'';nl}^{(i)}}{E_n^{(0)}-E_{n''}^{(0)}} - E_{nl}^{(2)}\,\frac{c_{nl';nl}^{(1)}}{E_{nl}^{(1)}-E_{nl'}^{(1)}}, \tag{5}$$

Its energy eigenvalues are given by $-x^3|V_2|^2/V_1$ and $xV_1 + x^3|V_2|^2/V_1$ up to $\mathcal{O}(x^3)$, and the corresponding eigenvectors are given by $(1, -xV_2^*/V_1)$ and $(xV_2/V_1, 1)$ up to $\mathcal{O}(x)$. The appearance of V_1 in the denominator signals enhanced contributions.

[3] For simplicity we neglect the electromagnetic interaction of quarks. In the case of bottom quark, numerically its effects are small even compared to the NNNLO corrections in α_s. The electric charge of bottom quark $Q_b = -1/3$ plays a role of an extra suppression factor in addition to the small QED coupling constant $\alpha \simeq 1/137$, as compared to, e.g., $\alpha_s(m_b) \simeq 0.23$.

$$d^{(2)}_{n'l';nl} = \langle n'l'|\, V^{(2)}\, |nl\rangle + \langle n'l'|\, V^{(1)}\, |nl'\rangle \frac{c^{(1)}_{nl';nl}}{E^{(1)}_{nl} - E^{(1)}_{nl'}} + \sum_{n''\neq n,\ l''} \langle n'l'|\, V^{(1)}\, |n''l''\rangle \frac{d^{(1)}_{n''l'';nl}}{E^{(0)}_{n} - E^{(0)}_{n''}} - E^{(1)}_{nl} \frac{d^{(1)}_{n'l';nl}}{E^{(0)}_{n} - E^{(0)}_{n'}}, \tag{6}$$

$$c^{(3)}_{nl';nl} = \langle nl'|\, V^{(4)}\, |nl\rangle + \sum_{i=1}^{2}\sum_{l''\neq l} \langle nl'|\, V^{(4-i)}\, |nl''\rangle \frac{c^{(i)}_{nl'';nl}}{E^{(1)}_{nl} - E^{(1)}_{nl''}} + \sum_{i=1}^{3}\sum_{n''\neq n,\ l''} \langle nl'|\, V^{(4-i)}\, |n''l''\rangle \frac{d^{(i)}_{n''l'';nl}}{E^{(0)}_{n} - E^{(0)}_{n''}} - \sum_{i=1}^{2} E^{(4-i)}_{nl} \frac{c^{(i)}_{nl';nl}}{E^{(1)}_{nl} - E^{(1)}_{nl'}}, \tag{7}$$

$$d^{(3)}_{n'l';nl} = \langle n'l'|\, V^{(3)}\, |nl\rangle + \sum_{i=1}^{2}\sum_{l''\neq l} \langle n'l'|\, V^{(3-i)}\, |nl''\rangle \frac{c^{(i)}_{nl'';nl}}{E^{(1)}_{nl} - E^{(1)}_{nl''}} + \sum_{i=1}^{2}\sum_{n''\neq n,\ l''} \langle n'l'|\, V^{(3-i)}\, |n''l''\rangle \frac{d^{(i)}_{n''l'';nl}}{E^{(0)}_{n} - E^{(0)}_{n''}} - \sum_{i=1}^{2} E^{(3-i)}_{nl} \frac{d^{(i)}_{n'l';nl}}{E^{(0)}_{n} - E^{(0)}_{n'}}. \tag{8}$$

Here, $E^{(k)}_{nl}$ denotes the coefficient of ε^k of E_{nlsj} [cf., eq. (2)], and it is understood that $c^{(i)}_{nl';nl} = 0$ if $l' = l$. As can be seen, an enhanced contribution proportional to $c^{(1)}_{nl';nl}/\left[E^{(1)}_{nl} - E^{(1)}_{nl'}\right]$ appears already at the first order for the wave function. A derivation of the perturbative expansions of E_{nlsj} and $|\Psi_{nlsj}\rangle$ is given in the appendix.

Physical quantities, such as the quark pair production cross section near threshold in e^+e^- collisions[4] and the quarkonium leptonic decay width, are proportional to the absolute square of the wave function at the origin, and the enhanced corrections to these observables arise from the second order. This is because only the S-wave ($l = 0$) wave functions have non-vanishing values at the origin, and since the enhanced corrections should connect different ls, namely they should be proportional to $|\langle n, l=0|\, V^{(2)}\, |n, l'\neq 0\rangle|^2$.

So far we have implicitly assumed that $\langle nl|\, V^{(2)}\, |nl'\rangle \neq 0$ for $l' \neq l$, but if this matrix element vanishes for some reasons, the enhanced corrections from quasi-degenerate states do not appear at least up to the fourth order in the energy level, as well as up to the third order in the quark pair production cross section (or quarkonium leptonic decay width).[5]

3. Vanishing off-diagonal matrix elements of $V^{(2)}$

In this section we evaluate the matrix element $\langle nl|\, V^{(2)}\, |nl'\rangle$ explicitly and show that it vanishes if $l' \neq l$.[6] The operator in $V^{(2)}$ which can have non-vanishing off-diagonal matrix elements for different ls is the so-called tensor operator

$$V^{(2)}_T = \frac{C_F \alpha_s}{4m^2 r^3} S_{12}, \qquad S_{12} = 2\left(3\frac{(\vec{r}\cdot\vec{S})^2}{r^2} - \vec{S}^2\right). \tag{9}$$

Its matrix element can be factorized into two parts:

$$\langle nlsj|\, V^{(2)}_T\, |nl'sj\rangle = \langle nl|\, \frac{C_F\alpha_s}{4m^2 r^3}\, |nl'\rangle\, \langle lsj|\, S_{12}\, |l'sj\rangle\,, \tag{10}$$

where the first factor represents the radial part and the second factor represents the angular and spin part.

The radial matrix has a form

$$\frac{C_F\alpha_s}{4m^2}\langle nl|\,\frac{1}{r^3}\,|nl'\rangle = \begin{array}{c} \begin{array}{cccccc} l'=0 & 1 & 2 & 3 & \cdots & n-1 \end{array} \\ \begin{pmatrix} \star & \star & 0 & 0 & \cdots & 0 \\ \star & \star & \star & 0 & \cdots & 0 \\ 0 & \star & \star & \star & \cdots & 0 \\ 0 & 0 & \star & \star & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \star \end{pmatrix} \end{array} \begin{array}{c} l=0 \\ 1 \\ 2 \\ 3 \\ \\ n-1 \end{array}, \tag{11}$$

where the star ($\star$) denotes a non-zero value. (This can easily be shown using the generating function for the Laguerre polynomial.) Namely, the radial matrix element vanishes in the case $|l - l'| \geq 2$.

On the other hand, because of the parity of S_{12} and the orbital wave function, S_{12} can mix the state of $l = j \pm 1$, $s = 1$ with $l' = j \pm 1$, $s = 1$, and of $l = j$, $s = 1$ with $l' = j$, $s = 1$. Other matrix elements vanish. By explicit computation the angular matrix elements are given by [17–19]

$$\langle lsj|\, S_{12}\, |l'sj\rangle = \begin{array}{c} \begin{array}{ccc} l'=j-1 & j & j+1 \end{array} \\ \begin{pmatrix} -\frac{2(j-1)}{2j+1} & 0 & \frac{6\sqrt{j(j+1)}}{2j+1} \\ 0 & 2 & 0 \\ \frac{6\sqrt{j(j+1)}}{2j+1} & 0 & -\frac{2(j+2)}{2j+1} \end{pmatrix} \end{array} \begin{array}{c} l=j-1 \\ l=j \\ l=j+1 \end{array} \qquad \text{for } s=1,\ j\geq 1, \tag{12}$$

[4] These corrections can make sense only in the close vicinity of distinct quasi-degenerate resonance peaks. Otherwise the enhancement from the small denominators is lost, for instance, by smearing due to the resonance widths.

[5] There is also a contribution from the D-wave production (or decay) via the higher-dimensional local current operator. In the case $\langle nl|\, V^{(2)}\, |nl'\rangle = 0$, contribution of enhanced corrections through such an operator also starts from the fourth-order correction.

[6] The vanishing of the matrix elements relies on the property of radial wave functions of Coulomb system $H_0 = p^2/m - C_F\alpha_s/r$. If one takes another wave function, for instance one in phenomenological potential models the matrix elements can have non-zero values, while it violates rigid order counting of pNRQCD and brings yet higher-order effects considered here into the computation of the matrix elements.

$$\langle lsj|\, S_{12}\, |l'sj\rangle = -4 \qquad \text{for } l = l' = 1, s = 1, j = 0, \tag{13}$$

and $\langle lsj|\, S_{12}\, |l'sj\rangle = 0$ otherwise. Thus, the only non-vanishing off-diagonal matrix elements are the ones with $|l - l'| = 2$.

Combining eqs. (11), (12), we obtain

$$\langle nlsj|\, V_T^{(2)}\, |nl'sj\rangle = \langle nl|\, \frac{C_F\alpha_s}{4m^2r^3}\, |nl'\rangle\, \langle lsj|\, S_{12}\, |l'sj\rangle = 0 \tag{14}$$

for all n, l, $l'(\neq l)$, s, j.

4. Enhanced corrections at higher orders

The analysis of the previous section does not apply to the tensor operator in the third-order potential,

$$V_T^{(3)} = \frac{C_F\alpha_s}{2m^2r^3}\frac{\alpha_s}{\pi}\left[\frac{1}{72}\Big\{C_A(97 + 18L_m - 18L_r) + 4(9C_F - 5T_F n_l)\Big\} + \frac{1}{24}\beta_0(3L_r - 8)\right] S_{12}, \tag{15}$$

where $L_m = \log(\mu^2/m^2)$, $L_r = \log(e^{2\gamma_E}\mu^2 r^2)$. The essential difference between $V_T^{(2)}$ and $V_T^{(3)}$ originates from the $\log r$ terms, resulting in non-zero radial matrix elements for $|l - l'| \geq 2$. Indeed the off-diagonal matrix elements of $\langle nlsj|\, V_T^{(3)}\, |nl'sj\rangle$ have non-zero values. It follows that the second order correction to the wave function $c^{(2)}$ in eq. (5) has non-zero values, as well as the cross-term of $\langle V^{(3-i)}\rangle$ and $d^{(i)}$ in eq. (8) also has nonzero values.

Up to this point we considered enhanced contributions from the intermediate states whose degeneracy is lifted by the order ε perturbation. Let us comment on contributions from the states whose degeneracy is lifted first at order ε^2, namely, from the multiplets of fine and hyperfine splittings [with the same (n, l) but different (s, j)]. Such contributions, if they exist, would give rise to more pronounced enhancement effects than those considered so far, since the level splittings which enter the denominator are order ε^2. In fact such contributions are absent to all orders in ε, since the transition matrix elements of $V^{(i)}$ between the states with the same (n, l) but different (s, j) vanish by parity and charge-parity conservation of QCD.[7] Thus, the order ε^2 quasi-degeneracy of the multiplets with the same (n, l) does not give enhanced contributions to either the energy level or the wave function.

Taking into account the fact that $c^{(1)} = 0$, $c^{(2)} \neq 0$ in eq. (3), the fourth- and fifth-order corrections to the energy level are given by

$$E_{nlsj}^{(4)} = \langle nl|\, V^{(4)}\, |nl\rangle + \sum_{i=1}^{3}\sum_{n'\neq n,\, l'} \frac{\langle nl|\, V^{(4-i)}\, |n'l'\rangle\, d^{(i)}_{n'l';nl}}{E_n^{(0)} - E_{n'}^{(0)}}, \tag{16}$$

$$E_{nlsj}^{(5)} = \langle nl|\, V^{(5)}\, |nl\rangle + \sum_{i=1}^{4}\sum_{n'\neq n,\, l'} \frac{\langle nl|\, V^{(5-i)}\, |n'l'\rangle\, d^{(i)}_{n'l';nl}}{E_n^{(0)} - E_{n'}^{(0)}} + \sum_{l'\neq l} \frac{\langle nl|\, V^{(3)}\, |nl'\rangle\, c^{(2)}_{nl';nl}}{E_{nl}^{(1)} - E_{nl'}^{(1)}}. \tag{17}$$

Note that the fourth-order correction does not contain the enhanced corrections from quasi-degeneracy, which can be seen from the absence of the c-term in eq. (16).

5. Conclusions

We have reconsidered the perturbation theory for the Schrödinger equation of the heavy quarkonium system in pNRQCD, taking into account contributions of quasi-degenerate states. As expected there are enhanced contributions which rearrange the order counting of the expansion. (In other words, it can be regarded as a question on the proper order counting of the l-changing mixing effects.) At the (naive) lowest order, the effect from the quasi-degenerate states is induced only from one type of off-diagonal matrix elements in the l-space, $\langle nlsj|\, V_T^{(2)}\, |nl'sj\rangle$. This matrix element vanishes, hence the quasi-degenerate correction vanishes at the naive lowest order. As a result this type of corrections is expected to appear first at the fifth order in the energy level and at the second order in the wave function. The contribution to the heavy quark threshold cross section or leptonic decay width is expected to start at the fourth order.

Thus, these specific corrections turn out to be irrelevant with respect to the current highest-level perturbative QCD calculations (energy levels and leptonic decay width at NNNLO). We think that this fact itself should be stated clearly. It should also be noted that, since the enhanced corrections to the wave function are expected to appear already at the second order, they may be important for other physical observables, such as level transition rates in certain channels. We also note that, even if the flavors of quark and antiquark are different (such as the B_c system), enhanced quasi-degenerate contributions to the NNNLO spectrum [21] (l-changing mixing) vanish similarly to the equal flavor case.[8] These subjects will be discussed separately.

We remark that if one had a sufficiently wide knowledge one could reach the same conclusion without any computation, since all the necessary results were available in the literature. In this sense there is hardly any truly new ingredient in the present work. We find, however, that it is not easy to collect these pieces of information together, in particular since the old results on perturbative computation of bound states before the advent of modern EFT are scattered through literature in an unorganized way. At least it would be meaningful to bring these results to the attention of experts at the forefront.

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[7] The parity and charge-parity of the heavy quarkonium system of the same flavor are given, respectively, by $P = (-1)^{l+1}$ and $C = (-1)^{l+s}$ [20]. Hence, variations of l and s, respectively, are allowed only by even numbers. Since $s = 0, 1$, this means s cannot change and l can change only by 0 or 2.

[8] In this case there are well-known mixing effects between different s states from the second-order energy levels, which correspond to the different diagonalizing basis for $V^{(2)}$ for the same (n, l).

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Appendix. General terms of perturbative series

In this appendix, we derive the general expressions for the energy level correction and the wave function correction at the N-th order, in the case that the degeneracy is lifted by the first-order and second-order corrections stepwise. The expressions shown in Secs. 2 and 4 are special cases of the general expressions eqs. (21), (23) and (25).

We expand the Schrödinger equation as

$$\left(H^{(0)}+\sum_{i=1}^{\infty}\varepsilon^i V^{(i)}\right)\left(\sum_{i'=0}^{\infty}\varepsilon^{i'}\left|\Psi_{nlsj}^{(i')}\right\rangle\right)=\left(\sum_{i=0}^{\infty}\varepsilon^i E_{nlsj}^{(i)}\right)\left(\sum_{i'=0}^{\infty}\varepsilon^{i'}\left|\Psi_{nlsj}^{(i')}\right\rangle\right). \tag{18}$$

The labels s and j are suppressed in the rest of this appendix. For notational simplicity, we redefine the wave function corrections as $\tilde{c}^{(i)}_{nl';nl}=c^{(i)}_{nl';nl}/(E^{(1)}_{nl}-E^{(1)}_{nl'})$ and $\tilde{d}^{(i)}_{n'l';nl}=d^{(i)}_{n'l';nl}/(E^{(0)}_{n}-E^{(0)}_{n'})$. Then the full wave function is given by

$$|\Psi_{nl}\rangle=\sum_{i=0}^{\infty}\varepsilon^i\left|\Psi_{nl}^{(i)}\right\rangle=|nl\rangle+\sum_{i=1}^{\infty}\sum_{l'\neq l}\varepsilon^i\,|nl'\rangle\,\tilde{c}^{(i)}_{nl';nl}+\sum_{i=1}^{\infty}\sum_{n'\neq n,\,l'}\varepsilon^i\,|n'l'\rangle\,\tilde{d}^{(i)}_{n'l';nl}. \tag{19}$$

In addition, we write $V^{(i)}_{n'l';nl}=\langle n'l'|\,V^{(i)}\,|nl\rangle$ in the following.

The coefficient of ε^N of the Schrödinger equation (18) reads

$$V^{(N)}\,|nl\rangle+\sum_{i=1}^{N-1}V^{(N-i)}\left|\Psi_{nl}^{(i)}\right\rangle+H^{(0)}\left|\Psi_{nl}^{(N)}\right\rangle=E_{nl}^{(N)}\,|nl\rangle+\sum_{i=1}^{N-1}E_{nl}^{(N-i)}\left|\Psi_{nl}^{(i)}\right\rangle+E_n^{(0)}\left|\Psi_{nl}^{(N)}\right\rangle. \tag{20}$$

The correction to the energy level is obtained by multiplying eq. (20) by $\langle nl|$ from the left. Since $\left\langle nl\,\middle|\,\Psi_{nl}^{(i)}\right\rangle=0$ for $i\geq 1$, the only remaining term on the right-hand side is $E_{nl}^{(N)}$. Then we obtain

$$E_{nl}^{(N)}=V^{(N)}_{nl;nl}+\sum_{i=1}^{N-1}\sum_{l''\neq l}V^{(N-i)}_{nl;nl''}\tilde{c}^{(i)}_{nl'';nl}+\sum_{i=1}^{N-1}\sum_{n''\neq n,\,l''}V^{(N-i)}_{nl;n''l''}\tilde{d}^{(i)}_{n''l'';nl}. \tag{21}$$

Next we consider the correction to the wave function. Multiplying eq. (20) by $\langle n'l'|$ from the left, we obtain

$$V^{(N)}_{n'l';nl}+\sum_{i=1}^{N-1}\sum_{l''\neq l}V^{(N-i)}_{n'l';nl''}\tilde{c}^{(i)}_{nl'';nl}+\sum_{i=1}^{N-1}\sum_{n''\neq n,\,l''}V^{(N-i)}_{n'l';n''l''}\tilde{d}^{(i)}_{n''l'';nl}+E^{(0)}_{n'}\tilde{d}^{(N)}_{n'l';nl}=\sum_{i=1}^{N-1}E^{(N-i)}_{nl}\tilde{d}^{(i)}_{n'l';nl}+E^{(0)}_{n}\tilde{d}^{(N)}_{n'l';nl}, \tag{22}$$

where $\tilde{d}^{(N)}_{n'l';nl}$ is separated outside the summation. Solving eq. (22) for $d^{(N)}_{n'l';nl}$, we obtain

$$d^{(N)}_{n'l';nl}=V^{(N)}_{n'l';nl}+\sum_{i=1}^{N-1}\sum_{l''\neq l}V^{(N-i)}_{n'l';nl''}\tilde{c}^{(i)}_{nl'';nl}+\sum_{i=1}^{N-1}\sum_{n''\neq n,\,l''}V^{(N-i)}_{n'l';n''l''}\tilde{d}^{(i)}_{n''l'';nl}-\sum_{i=1}^{N-1}E^{(N-i)}_{nl}\tilde{d}^{(i)}_{n'l';nl}. \tag{23}$$

Note that the left-hand-side of eq. (23) is not $\tilde{d}^{(N)}_{n'l';nl}$ but $d^{(N)}_{n'l';nl}$.

The case with $\tilde{c}^{(N)}_{nl';nl}$ is similar to that of $\tilde{d}^{(N)}_{n'l';nl}$ except that we first need to replace $N\to N+1$ in eq. (20). Then multiplying it by $\langle nl'|$ from the left, we obtain

$$V^{(N+1)}_{nl';nl}+\sum_{i=1}^{N-1}\sum_{l''\neq l}V^{(N-i+1)}_{nl';nl''}\tilde{c}^{(i)}_{nl'';nl}+E^{(1)}_{nl'}\tilde{c}^{(N)}_{nl';nl}+\sum_{i=1}^{N}\sum_{n''\neq n,\,l''}V^{(N-i+1)}_{nl';n''l''}\tilde{d}^{(i)}_{n''l'';nl}=\sum_{i=1}^{N-1}E^{(N-i+1)}_{nl}\tilde{c}^{(i)}_{nl';nl}+E^{(1)}_{nl}\tilde{c}^{(N)}_{nl';nl}. \tag{24}$$

Solving for $c^{(N)}_{nl';nl}$, we obtain

$$c^{(N)}_{nl';nl}=V^{(N+1)}_{nl';nl}+\sum_{i=1}^{N-1}\sum_{l''\neq l}V^{(N-i+1)}_{nl';nl''}\tilde{c}^{(i)}_{nl'';nl}+\sum_{i=1}^{N}\sum_{n''\neq n,\,l''}V^{(N-i+1)}_{nl';n''l''}\tilde{d}^{(i)}_{n''l'';nl}-\sum_{i=1}^{N-1}E^{(N-i+1)}_{nl}\tilde{c}^{(i)}_{nl';nl}. \tag{25}$$

Again we note the difference between c and $\tilde{c}$, $\tilde{d}$ on both sides.

Thus, we obtain the energy level correction (21) and wave function correction (23), (25) at the N-th order in a recursive form.

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