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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 $H^{(0)}, V^{(1)}, \dots$ 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

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

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

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

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

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., $\alpha_s(m_b) \simeq 0.23$.