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2-Loop Quarkonium Hamiltonian (Non-annihilation channel)

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Heavy quarkonium system provides an ideal laboratory to investigate QCD deeply. We report on our calculation of the two-loop quarkonium Hamiltonian (in the non-annihilation channel). This is the first non-trivial calculation of the N^4LO corrections to the quarkonium Hamiltonian, defined in the potential-NRQCD effective field theory. We explain the procedure of this computation as well as theoretically interesting points, and then we present the result.

Loops and Legs in Quantum Field Theory (LL2024)
14-19, April, 2024
Wittenberg, Germany

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PoS(LL2024)020

The heavy quarkonium system has been an ideal tool to study deep aspects of QCD [1, 2]. In particular, it has been used to determine the fundamental physical constants such as m_c, m_b, and α_s [3]. In the future, it is expected that m_t will also be determined with a high precision using the cross section for $e^+e^- \to t\bar{t}$ in the threshold region [4]. The singlet Hamiltonian within the potential Nonrelativistic QCD (pNRQCD) effective field theory (EFT) [5] plays the principal role in these studies. In the leading order (LO) the Hamiltonian is simply that of a non-relativisitic quantum mechanical system with the Coulomb attractive force. Enormous efforts have been devoted to compute the higher-order corrections to the Hamiltonian systematically. This was enabled by the development of the EFTs such as pNRQCD and of the expansion-by-regions (EBR) technique [6]. The Hamiltonian has been known up to the next-to-next-to-next-to-leading order ($\mathrm{N^3LO}$) accuracy for more than a decade [7, 8], and it took roughly a decade to calculate the $\mathrm{N^3LO}$ Hamiltonian after $\mathrm{N^2LO}$ Hamiltonian was completed [9]. Certainly it is worthwhile to start calculations of the Hamiltonian at $\mathrm{N^4LO}$ accuracy. In addition, there is a theoretically interesting aspect of this calculation, to confirm whether the assumption of pNRQCD EFT on a specific form of the Hamiltonian is correct.

We report on our recent calculation of a part of the $\mathrm{N^4LO}$ quarkonium Hamiltonian [10]. This is done by the direct matching of the on-shell scattering amplitude between a heavy quark Q and a heavy antiquark $\bar{Q}$ calculated in full QCD and that calculated in pNRQCD EFT. This matching is carried out at the two-loop level and up to $O(\beta^0)$ in the non-relativistic expansion [relative $O(\alpha_s^2\beta^2)$ compared to the LO $\sim \alpha_s/\beta^2$ contribution], where β denotes the velocity of Q or $\bar{Q}$ in the center-of-mass (c.m.) frame.

In pNRQCD EFT, each term of the Hamiltonian, given as a quantum mechanical operator, is assumed to take a form $f(\hat{\vec{p}})V(r)g(\vec{S})$, where $f(\vec{p})$ is regular in $\hat{\vec{p}} = -i\vec{\nabla}$, $V(r)$ includes singularities such as $1/r$ or $\log r$, and $g(\vec{S})$ is regular in the quarkonium spin $\vec{S}$. In momentum space, the corresponding matrix element of the operator takes the form $\tilde{f}(\vec{p}, \vec{p}+\vec{k})\tilde{V}(|\vec{k}|)g(\vec{S})$, where $\tilde{f}, g$ are regular and $\tilde{V}$ is singular. On the other hand, the structure of the QCD $Q\bar{Q}$ scattering amplitude for $Q(\vec{p}) + \bar{Q}(-\vec{p}) \to Q(\vec{p}+\vec{k}) + \bar{Q}(-\vec{p}-\vec{k})$ is much more complicated, even after the expansion in β. (1) Although the amplitude is regular at $u = \vec{k}^2 - 4\vec{p}^{\,2} = 0$ in the physical sheet, it has singularities at $u = 0$ in the second and other Riemann sheets by analytical continuation. [An example of such a structure is $\log(4\vec{p}^{\,2}/\vec{k}^2)/(\vec{k}^2 - 4\vec{p}^{\,2})$.] (2) The contributions from the potential region in the EBR method include non-elementary functions of $|\vec{p}|/|\vec{k}|$ (counted as order one in the β expansion). Thus, it seems fairly non-trivial that the Hamiltonian takes such a simple form, from the viewpoint of the direct matching procedure. Up to now, the complete analytic expression of the $Q\bar{Q}$ scattering amplitude in full QCD is missing at the two-loop level. Hence, we aim to calculate its non-relativistic expansion, namely the expansion in β.

To reduce the labor of the calculation, we compute only the contributions from the non-annihilation channel of the heavy quark and antiquark, in this first calculation. To ensure theoretical consistency we consider the $\mathrm{SU}(N_C)$ gauge theory with n_h heavy quark flavors (each with the same mass m) and n_l massless quark flavors. (For convenience we call this theory as QCD.) We calculate the scattering amplitude between a heavy quark Q and a heavy antiquark $\bar{Q}'$ of different flavors (with mass m). In this case only diagrams in the non-annihilation channel contribute.

Our calculational procedure for the QCD scattering amplitude goes as follows.

(i) We project the scattering amplitude to a spinor basis, by which the coefficients of the spinor basis are expressed by scalar loop integrals.

(ii) We perform integration-by-parts (IBP) reduction [11] of the scalar integrals. Using the program `Kira` [12] for the reduction, all the coefficients are expressed by 149 master integrals (MIs).

(iii) We expand each MI in β. For this purpose, we use the differential equation [13] satisfied by MIs, which is an exact equation. This is supplemented by the EBR technique, used to determine the boundary conditions in solving the differential equation.

Let us explain more details.

(i) The scattering amplitude for $Q(p)+\bar{Q}'(\bar{p}) \to Q(p')+\bar{Q}'(\bar{p}')$ can be expressed by a linear combination of the following types of spinor structure after loop integration:

$$[\bar{u}(p')\gamma^{\alpha_1}\cdots\gamma^{\alpha_n}u(p)]\cdot\left[\bar{v}(\bar{p})\gamma_{\alpha_n}\cdots\gamma_{\alpha_1}v(\bar{p}')\right], \tag{1}$$
$$[\bar{u}(p')\bar{p}\cdot\gamma\,\gamma^{\alpha_1}\cdots\gamma^{\alpha_n}u(p)]\cdot\left[\bar{v}(\bar{p})\gamma_{\alpha_n}\cdots\gamma_{\alpha_1}v(\bar{p}')\right], \tag{2}$$
$$[\bar{u}(p')\gamma^{\alpha_1}\cdots\gamma^{\alpha_n}u(p)]\cdot\left[\bar{v}(\bar{p})\gamma_{\alpha_n}\cdots\gamma_{\alpha_1}p\cdot\gamma\,v(\bar{p}')\right], \tag{3}$$
$$[\bar{u}(p')\bar{p}\cdot\gamma\,\gamma^{\alpha_1}\cdots\gamma^{\alpha_n}u(p)]\cdot\left[\bar{v}(\bar{p})\gamma_{\alpha_n}\cdots\gamma_{\alpha_1}p\cdot\gamma\,v(\bar{p}')\right]. \tag{4}$$

The 2-loop amplitude can be expressed with a 21-dimensional basis. The coefficients of the basis can be expressed by scalar integrals, after projecting the loop amplitudes to the spinor basis and using the standard trace technology of the gamma matrices. Feynman integrals are regularized by dimensional regularization, where the number of the space-time dimensions is set to $4-2\epsilon$.

The above basis can be easily expressed by a two-component spinor basis in dimensional regularization. We adopt a 21-dimensional basis $\{\Lambda_1,\ldots,\Lambda_{21}\}$, where the first five elements are chosen as (apart from the initial and final state spinor wave functions)

$$\begin{aligned}
\Lambda_1 &= \mathbb{I}\otimes\mathbb{I}\,,\\
\Lambda_2 &= \sigma^a\,\sigma^b\otimes\sigma^a\,\sigma^b\,,\\
\Lambda_3 &= \sigma^a\,\sigma^b\,\sigma^c\,\sigma^d\otimes\sigma^a\,\sigma^b\,\sigma^c\,\sigma^d\,,\\
\Lambda_4 &= \frac{1}{m^2}\left(\vec{\sigma}\cdot\vec{k}\,\sigma^a\otimes\vec{\sigma}\cdot\vec{k}\,\sigma^a\right),\\
\Lambda_5 &= \frac{1}{m^2}\left(\vec{\sigma}\cdot\vec{p}\,'\,\vec{\sigma}\cdot\vec{p}\otimes\mathbb{I}+\mathbb{I}\otimes\vec{\sigma}\cdot\vec{p}\,'\,\vec{\sigma}\cdot\vec{p}\right).
\end{aligned} \tag{5}$$

The Pauli matrices satisfy

$$\{\sigma^i,\sigma^j\}=2\delta^{ij}\mathbb{I}\,,\quad \delta^{ii}=3-2\epsilon\,,\quad \mathrm{tr}\,\mathbb{I}=2\,. \tag{6}$$

m denotes the pole mass of the heavy quarks, and the amplitude is renormalized in the on-shell scheme.

(ii) IBP reduction is nowadays the standard procedure and we skip its explanation.

(iii) EBR is a technique to obtain the expansion of a loop integral in a small parameter (in our case β) by decomposing the loop integral into a sum of contributions from different regions in dimensional regularization. Each MI can be regarded as a sum of the contributions from the

7 regions: HH, HS, HP, SS, SP, PP, and PUS, in terms of the EBR language (H: hard, S: soft, P: potential, US: ultra-soft). We can group them into 4 regions as HH, HS+HP, SS+SP+PP and PUS. Then, the MIs corresponding to each of the 4 regions satisfy the differential equation by themselves. We solve the differential equation order by order in expansion in β corresponding to each region, where the boundary conditions for the MIs are determined by calculating the LO terms of the β expansions using the EBR technique. (In some cases, the boundary condition can be fixed by demanding the MI to be regular at $u = 0$ in the physical sheet.) This method is much more economical as compared to calculating the β expansions of the MIs or diagrams by only the EBR technique. As a result, each MI is obtained, after combining the contributions from all the regions, in the form

$$\mathrm{MI} = \sum_{r\in\text{regions}} \sum_{j} (\text{EBR MI})_{rj} \times \left[1 + \sum_{2n+l\geq 1} C_{nl}^{rj} \left(\frac{|\vec{p}|^2}{m^2}\right)^n \left(\frac{|\vec{k}|}{m}\right)^l\right], \tag{7}$$

where $(\text{EBR MI})_{rj}$ denotes the jth MI belonging to each region r obtained after the expansion; $\vec{p}$ and $\vec{p}' = \vec{p} + \vec{k}$ denote, respectively, the three-momenta of the initial and final Q in the c.m. frame. ($|\vec{p}|^2 = |\vec{p}\,'|^2$ by the energy conservation.)

The calculational procedure for the scattering amplitude for the same process in pNRQCD EFT is similar. The amplitude is projected on to the two-component spinor basis. The scalar integrals are reduced to master integrals of the EFT using the integration-by-parts identities. After matching the amplitude to that of QCD, we readily obtain the two-loop Hamiltonian in the β expansion. The Hamiltonian up to $O(\beta^0)$ consists only of the five operators $\Lambda_1, \ldots, \Lambda_5$ of the spinor basis before expansion in ϵ, where the coefficients of the other operators vanish.

We have performed the following cross checks:

(1) We reproduced the known two-loop static QCD potential $V_{\rm QCD}^{(2\text{ loop})}$ [9] and two-loop $1/(mk)$ potential $V_{1/(mk)}^{(2\text{ loop})}$ [14] as part of the two-loop Hamiltonian. We also reproduced the known one-loop part of the N^{3}LO Hamiltonian [7] at an intermediate stage of the calculation.

(2) We checked that the QCD scattering amplitude is regular at $u = 0$ in the physical sheet.[1] Although we imposed the regularity at $u = 0$ on MIs, the regularity for the scattering amplitude is not trivial because the coefficients of the MIs include poles at $u = 0$.

(3) The two-loop Hamiltonian is regular in $\vec{p}$ but singular in $k = |\vec{k}|$. Each term of the Hamiltonian takes the form $f(\vec{p})V(k)g(\vec{S})$, where f and g are polynomials and $V(k)$ is proportional to $k^{a+b\epsilon}$ with $a \in \{-2, -1, 0\}$, $b \in \{-4, -2, 0\}$, before expansion in ϵ. This form is expected as originating from the hard (H) and soft (S) contributions according to the EBR technique and is consistent with the concept of the EFT construction. This means that all the singularities at $u = 0$ in the second and other Riemann sheets cancel between the scattering amplitudes of QCD and pNRQCD EFT. Additionally, the functions of p/k (P contributions) also cancel out.

Does this confirm correctness of the assumption of pNRQCD EFT for the form of the Hamiltonian up to two loops? — *Not quite,* since we used the EBR technique to determine the boundary

[1] The regularity of the amplitude at $u = 0$ in the physical sheet follows from the flavor conservation of QCD.

conditions for many of the MIs. There is always a logical possibility that we missed contributions from any regions which are not covered by our current knowledge of the EBR technique.

To compensate for this shortcoming, we evaluated the coefficients of the expansion in ϵ of each QCD master integral by numerical integrations (in part using `FIESTA` [15]) in the non-relativistic region. We compared them with the expansion of the master integral in β and ϵ obtained analytically and checked consistency. Furthermore, some of the ϵ expansions of the master integrals are known analytically [16, 17]. We expanded the analytical expressions in β and found agreement with our results. Consequently, up to the accuracy of the numerical tests, we confirm that the form of the Hamiltonian is very likely to be correct up to two loops.

Let us present our final result. We expand the coefficients of $\Lambda_1, \ldots, \Lambda_5$ in ϵ while we ignore any $O(\epsilon)$ contributions in Λ_i. (Namely, we simply take the limit $\epsilon \to 0$ for Λ_i.) The Hamiltonian is given in the form

$$H = \frac{16\pi^2 C_F}{k^2} \sum_{i=1}^{4} \sum_{j=1}^{3} \sum_{n,\ell \geq 0} \left(\frac{\alpha_s(k)}{4\pi}\right)^j C_{\{i,j,n,2\ell\}} \left(\frac{k}{m}\right)^n \frac{(p^2)^\ell + (p'^2)^\ell}{2\, m^{2\ell}} O_i \,, \tag{8}$$

where

$$k = \left|\vec{k}\right|, \quad p^2 = |\vec{p}|^2 \,, \quad p'^2 = |\vec{p}\,'|^2 \,, \quad \vec{p}\,' = \vec{p} + \vec{k} \,. \tag{9}$$

We absorb $\log(\mu/k)$ terms originating from the running of α_s by expressing the Hamiltonian by $\alpha_s(k)$, the strong coupling constant in the $\overline{\rm MS}$ scheme of the theory with n_l flavors only,[2,3] renormalized at $\mu = k$. The spinor basis in three dimensions is defined as

$$O_1 = \mathbb{I} \otimes \mathbb{I}, \;\; O_2 = \vec{S}^2 \,, \;\; O_3 = \frac{i}{k^2} \vec{S} \cdot \left(\vec{p} \times \vec{k}\right) \,, \;\; O_4 = \sigma^a \otimes \sigma^a - \frac{3}{k^2} \left(\vec{k} \cdot \vec{\sigma}\right) \otimes \left(\vec{k} \cdot \vec{\sigma}\right) \,, \tag{10}$$

with

$$\vec{S} = \frac{\vec{\sigma}}{2} \otimes \mathbb{I} + \mathbb{I} \otimes \frac{\vec{\sigma}}{2} \,. \tag{11}$$

The Wilson coefficients are separated into finite and divergent parts as

$$C_{\{i,j,n,2\ell\}} = C^{\rm fin}_{\{i,j,n,2\ell\}} + C^{\rm div}_{\{i,j,n,2\ell\}} \,. \tag{12}$$

2-loop non-zero finite Wilson coefficients are given by

$$\begin{aligned} C^{\rm fin}_{\{1,3,0,0\}} &= V^{(2\,\rm loop)}_{\rm QCD}(k) \left[C_F \alpha_s(k)^3/(4\pi k^2)\right]^{-1} \\ &= -\frac{100 n_l^2}{81} + n_l \left(\left(\frac{28\zeta(3)}{3} + \frac{899}{81}\right) C_A + \left(\frac{55}{6} - 8\zeta(3)\right) C_F\right) \\ &\quad + \left(-\frac{22\zeta(3)}{3} - \frac{4343}{162} - 4\pi^2 + \frac{\pi^4}{4}\right) C_A^2 \,, \end{aligned} \tag{13}$$

[2] In expressing the Hamiltonian, it is customary to rewrite the coupling constant of the full theory $\alpha_s^{(n_h+n_l)}(\mu)$ by that of the theory with n_l flavors only $\alpha_s(\mu) \equiv \alpha_s^{(n_l)}(\mu)$. We include the $O(\epsilon)$ term in this decoupling relation [18, 19], which simplifies the result slightly since the one-loop Hamiltonian includes the $1/\epsilon$ pole.

[3] We do not include the $O(\epsilon)$ correction to the running formula

$$\alpha_s(k) = \alpha_s(\mu) - \frac{\alpha_s(\mu)^2}{4\pi} \left(\frac{11}{3} C_A - \frac{2}{3} n_l\right) \log\left(\frac{k^2}{\mu^2}\right) + \cdots \,.$$

$$
\begin{aligned}
C^{\rm fin}_{\{1,3,1,0\}} &= V^{(2\ \rm loop)}_{1/(mk)}(k)\,[C_F\alpha_s(k)^3/(4\pi mk)]^{-1} \\
&= \left(-\frac{32}{3}\pi^2 C_A C_F - \frac{16}{3}\pi^2 C_A^2\right)\log\left(\frac{\mu^2}{k^2}\right) + n_l\left(\frac{49\pi^2 C_A}{18} - \frac{4\pi^2 C_F}{9}\right) \\
&\quad + \left(\frac{130\pi^2}{9} - \frac{32}{3}\pi^2\log(2)\right)C_A C_F + \left(-\frac{101\pi^2}{9} - \frac{16}{3}\pi^2\log(2)\right)C_A^2\,, \qquad (14)
\end{aligned}
$$

$$
\begin{aligned}
C^{\rm fin}_{\{1,3,2,0\}} &= \log^2\left(\frac{k^2}{m^2}\right)\left(-\frac{11C_A C_F}{9} + \frac{13C_A n_l}{9} - \frac{193C_A^2}{18} - \frac{2C_F n_l}{9}\right) \\
&\quad + \log\left(\frac{k^2}{m^2}\right)\left(-2\pi^2 C_F^2 + \left(\frac{146}{9} + \frac{13\pi^2}{9}\right)C_A C_F - \frac{17C_A n_h}{18} + \frac{637C_A n_l}{54}\right. \\
&\qquad \left. + \left(-\frac{304}{9} - \frac{14\pi^2}{9}\right)C_A^2 - \frac{340C_F n_l}{27}\right) \\
&\quad + \log\left(\frac{m^2}{\mu^2}\right)\left(\left(\frac{416}{9} - \frac{13\pi^2}{9}\right)C_A C_F + \frac{40C_A n_l}{9} - \frac{80C_F n_l}{9} - 4\pi^2 C_F^2\right. \\
&\qquad \left. + \left(-\frac{208}{9} - \frac{16\pi^2}{9}\right)C_A^2\right) \\
&\quad + \log(2)\left(22\pi^2 C_A C_F - 9\pi^2 C_A^2 - 6\pi^2 C_F^2\right) + \left(\frac{103\zeta(3)}{2} - \frac{407}{6} + \frac{13\pi^2}{24} + \frac{3\pi^4}{16}\right)C_A^2 \\
&\quad + \left(-77\zeta(3) + \frac{2369}{9} - \frac{713\pi^2}{54}\right)C_A C_F + \left(33\zeta(3) - \frac{946}{9} + \frac{6023\pi^2}{108}\right)C_F^2 + \frac{8n_h n_l}{27} \\
&\quad + \left(\frac{1387}{108} - \frac{41\pi^2}{36}\right)C_A n_h + \left(\frac{173\pi^2}{54} - \frac{346}{9}\right)C_F n_h + \left(\frac{28\pi^2}{27} - \frac{173}{27}\right)C_A n_l \\
&\quad + \left(\frac{424}{27} - \frac{8\pi^2}{27}\right)C_F n_l\,, \qquad (15)
\end{aligned}
$$

$$
\begin{aligned}
C^{\rm fin}_{\{1,3,0,2\}} &= \log\left(\frac{k^2}{\mu^2}\right)\left(\left(\frac{416}{9} + \frac{32\pi^2}{9}\right)C_A^2 - \frac{80C_A n_l}{9}\right) + \left(\frac{28\zeta(3)}{3} + \frac{1571}{81} - \frac{4\pi^2}{27}\right)C_A n_l \\
&\quad + \left(\frac{55}{6} - 8\zeta(3)\right)C_F n_l - \frac{100n_l^2}{81} + \left(-\frac{38\zeta(3)}{3} - \frac{7919}{162} + \frac{266\pi^2}{27} - \frac{\pi^4}{4}\right)C_A^2\,, \qquad (16)
\end{aligned}
$$

$$
\begin{aligned}
C^{\rm fin}_{\{2,3,2,0\}} &= \log^2\left(\frac{k^2}{m^2}\right)\left(\frac{38C_A^2}{9} - \frac{5C_A n_l}{9}\right) + \log\left(\frac{m^2}{\mu^2}\right)\left(\frac{8}{3}\pi^2 C_A C_F + \frac{4}{3}\pi^2 C_F^2\right) \\
&\quad + \log\left(\frac{k^2}{m^2}\right)\left(-\frac{46C_A C_F}{9} - \frac{82C_A n_l}{27} + \left(\frac{256}{27} - \frac{4\pi^2}{9}\right)C_A^2 + \frac{16C_F n_l}{9}\right) \\
&\quad + \log(2)\left(12\pi^2 C_F^2 - \frac{238}{9}\pi^2 C_A C_F + \frac{71}{9}\pi^2 C_A^2\right) + \left(\frac{16\pi^2}{27} - \frac{538}{81}\right)C_A n_h \\
&\quad + \left(\frac{596}{27} - \frac{16\pi^2}{9}\right)C_F n_h + \frac{100n_l^2}{243} + \left(-18\zeta(3) - \frac{10}{3} - \frac{239\pi^2}{9}\right)C_F^2 \\
&\quad + \left(-\frac{295\zeta(3)}{18} + \frac{11651}{486} - \frac{127\pi^2}{27} - \frac{\pi^4}{12}\right)C_A^2 + \left(-\frac{13\zeta(3)}{3} - \frac{70}{27} + \frac{170\pi^2}{9}\right)C_A C_F \\
&\quad + \left(-\frac{28\zeta(3)}{9} - \frac{503}{243} - \frac{10\pi^2}{27}\right)C_A n_l + \left(\frac{8\zeta(3)}{3} - \frac{637}{54}\right)C_F n_l\,, \qquad (17)
\end{aligned}
$$

$$
\begin{aligned}
C^{\rm fin}_{\{3,3,2,0\}} &= \log\left(\frac{k^2}{m^2}\right)\left(\frac{56C_AC_F}{3}-\frac{70C_An_l}{9}+\frac{262C_A^2}{9}-\frac{8C_Fn_l}{3}\right)\\
&+\log^2\left(\frac{k^2}{m^2}\right)\left(\frac{14C_A^2}{3}-\frac{2C_An_l}{3}\right)+\log(2)\left(\frac{8}{3}\pi^2C_AC_F+\frac{8}{3}\pi^2C_A^2-16\pi^2C_F^2\right)\\
&+\left(3\zeta(3)+\frac{5999}{108}-\frac{4\pi^2}{9}-\frac{3\pi^4}{8}\right)C_A^2+\left(\frac{10\pi^2}{9}-\frac{298}{27}\right)C_An_h+\left(\frac{476}{9}-\frac{16\pi^2}{3}\right)C_Fn_h\\
&+\frac{50n_l^2}{27}+\left(-14\zeta(3)-\frac{827}{54}-\frac{4\pi^2}{9}\right)C_An_l+\left(-4\zeta(3)+\frac{590}{9}+\frac{8\pi^2}{3}\right)C_AC_F\\
&+\left(12\zeta(3)-\frac{1055}{36}\right)C_Fn_l+\left(24\zeta(3)-62+\frac{40\pi^2}{3}\right)C_F^2\,, \qquad (18)\\
C^{\rm fin}_{\{4,3,2,0\}} &= \log\left(\frac{k^2}{m^2}\right)\left(\frac{17C_AC_F}{9}-\frac{35C_An_l}{54}+\frac{149C_A^2}{54}-\frac{2C_Fn_l}{9}\right)\\
&+\log^2\left(\frac{k^2}{m^2}\right)\left(\frac{17C_A^2}{36}-\frac{C_An_l}{18}\right)+\log(2)\left(\frac{2}{9}\pi^2C_AC_F+\frac{2}{9}\pi^2C_A^2-\frac{4}{3}\pi^2C_F^2\right)\\
&+\left(-\frac{\zeta(3)}{18}+\frac{12299}{1944}+\frac{\pi^2}{18}-\frac{\pi^4}{48}\right)C_A^2+\left(\frac{5\pi^2}{54}-\frac{149}{162}\right)C_An_h+\left(\frac{119}{27}-\frac{4\pi^2}{9}\right)C_Fn_h\\
&+\frac{25n_l^2}{243}+\left(-\frac{7\zeta(3)}{9}-\frac{1367}{972}-\frac{\pi^2}{27}\right)C_An_l+\left(-\frac{\zeta(3)}{3}+\frac{331}{54}+\frac{2\pi^2}{9}\right)C_AC_F\\
&+\left(\frac{2\zeta(3)}{3}-\frac{445}{216}\right)C_Fn_l+\left(2\zeta(3)-\frac{29}{6}+\frac{10\pi^2}{9}\right)C_F^2\,. \qquad (19)
\end{aligned}
$$

2-loop non-zero divergent Wilson coefficients are given by

$$
\begin{aligned}
C^{\rm div}_{\{1,3,1,0\}} &= -\frac{8\pi^2C_A^2}{3\epsilon}-\frac{16\pi^2C_AC_F}{3\epsilon}\,, \qquad (20)\\
C^{\rm div}_{\{1,3,2,0\}} &= \log\left(\frac{k^2}{\mu^2}\right)\left(-\frac{88C_AC_F}{9\epsilon}-\frac{8C_An_l}{9\epsilon}+\frac{44C_A^2}{9\epsilon}+\frac{16C_Fn_l}{9\epsilon}\right)\\
&+\left(\frac{44}{9\epsilon^2}+\frac{13\pi^2}{18\epsilon}-\frac{208}{9\epsilon}\right)C_AC_F+\left(-\frac{22}{9\epsilon^2}+\frac{8\pi^2}{9\epsilon}+\frac{104}{9\epsilon}\right)C_A^2+\frac{2\pi^2C_F^2}{\epsilon}\\
&+\left(\frac{4}{9\epsilon^2}-\frac{20}{9\epsilon}\right)C_An_l+\left(\frac{40}{9\epsilon}-\frac{8}{9\epsilon^2}\right)C_Fn_l\,, \qquad (21)\\
C^{\rm div}_{\{1,3,0,2\}} &= \log\left(\frac{k^2}{\mu^2}\right)\left(\frac{16C_An_l}{9\epsilon}-\frac{88C_A^2}{9\epsilon}\right)+\left(\frac{44}{9\epsilon^2}-\frac{16\pi^2}{9\epsilon}-\frac{208}{9\epsilon}\right)C_A^2\\
&+\left(\frac{40}{9\epsilon}-\frac{8}{9\epsilon^2}\right)C_An_l\,, \qquad (22)\\
C^{\rm div}_{\{2,3,2,0\}} &= -\frac{4\pi^2C_AC_F}{3\epsilon}-\frac{2\pi^2C_F^2}{3\epsilon}\,. \qquad (23)
\end{aligned}
$$

The color factors are given by $C_F = (N_C^2-1)/(2N_C)$ and $C_A = N_C$ for the SU(N_C) gauge group.

In summary we computed the quarkonium Hamiltonian at the two-loop level in the non-annihilation channel. The obtained Hamiltonian has an expected form as resulting from integrating

the H and S modes. The developed calculational procedure, combining the differential equation and EBR technique, is useful to compute the β expansion of the scattering amplitude.

For a consistent calculation of physical observables at N^{4}LO accuracy using the Hamiltonian, it is sometimes required to include higher-order terms of β and ϵ at the tree and one-loop levels than those given in the literature. We provide them in the Appendix.

Acknowledgement

This work is done in collaboration with G. Mishima and H. Takaura. The work was supported in part by JSPS KAKENHI Grant Numbers JP23K03404.

A. Tree-level and one-loop Hamiltonians

We present the tree-level and one-loop Hamiltonians before expanding in ϵ, up to $O(\beta^2)$ and $O(\beta)$ [$O(\beta^4)$ and $O(\alpha_s\beta^3)$ relative to the LO], respectively. The Hamiltonian is given in the form

$$H = \frac{C_F\,\bar{\mu}^{-2\epsilon}}{k^2} \sum_{i=1}^{6} \sum_{j=1}^{3} \sum_{n,\ell\geq 0} \left(g_R^2\,\bar{\mu}^{2\epsilon}\right)^j W_{\{i,j,n,2\ell\}} \left(\frac{k}{m}\right)^n \frac{(p^2)^\ell + (p'^2)^\ell}{2\,m^{2\ell}}\,\Lambda_i\,. \tag{24}$$

$g_R = \sqrt{4\pi\alpha_s^{(n_h+n_l)}(\mu)}$ denotes the renormalized gauge coupling constant in the $\overline{\rm MS}$ scheme of the full theory (with n_h heavy quark flavors and n_l massless quark flavors); $\bar{\mu}^2 = \mu^2\,e^{\gamma_E}/(4\pi)$. The spinor basis is defined in eq. (5) and in addition one more spinor structure is necessary at the tree level $O(\beta^2)$:

$$\Lambda_6 = \frac{1}{m^4}\,(\vec{\sigma}\cdot\vec{p}'\,\vec{\sigma}\cdot\vec{p}\otimes\vec{\sigma}\cdot\vec{p}'\,\vec{\sigma}\cdot\vec{p})\ .$$

We list only those Wilson coefficients which are non-zero.

At tree level and up to $O(\beta^4)$ relative to LO, they are given by

$$\begin{aligned} &W_{\{1,1,0,0\}} = -1, \quad W_{\{1,1,0,2\}} = \frac{1}{2}\,, \quad W_{\{1,1,0,4\}} = -\frac{7}{16}\,, \quad W_{\{4,1,0,0\}} = -\frac{1}{4}, \\ &W_{\{4,1,0,2\}} = \frac{1}{4}\,, \quad W_{\{5,1,0,0\}} = -\frac{3}{4}\,, \quad W_{\{5,1,0,2\}} = \frac{3}{4}\,, \quad W_{\{6,1,0,0\}} = -\frac{1}{16}\,. \end{aligned} \tag{25}$$

At one loop and up to $O(\alpha_s\beta^3)$ relative to LO, the Wilson coefficients are given by

$$\begin{aligned} W_{\{1,2,0,0\}} &= m^{-2\epsilon}\cdot\frac{2}{3}(\epsilon-1)n_h\,iI_H - \bar{\mu}^{-2\epsilon}\cdot 2\,\delta_1 Z_g \\ &\quad + k^{-2\epsilon}\left(-\frac{(\epsilon-1)(8\epsilon-11)C_A}{2\epsilon-3} - \frac{2(\epsilon-1)n_l}{2\epsilon-3}\right) iI_S^a\,, \end{aligned} \tag{26}$$

$$W_{\{1,2,1,0\}} = k^{-2\epsilon}\left((\epsilon-1)C_A - \frac{1}{2}(2\epsilon-1)C_F\right) iI_S^b\,, \tag{27}$$

$$\begin{aligned} W_{\{1,2,2,0\}} &= m^{-2\epsilon}\left(-\frac{(\epsilon-1)\left(96\epsilon^3-100\epsilon^2+12\epsilon-29\right)C_A}{24(2\epsilon-1)(2\epsilon+1)}\right. \\ &\quad \left. + \frac{(\epsilon-1)\left(96\epsilon^4+44\epsilon^3-96\epsilon^2+37\epsilon+6\right)C_F}{6(2\epsilon-1)(2\epsilon+1)(2\epsilon+3)} - \frac{2}{15}\epsilon(\epsilon-1)n_h\right) iI_H \\ &\quad + k^{-2\epsilon}\left(\frac{1}{24}\left(-48\epsilon^2+104\epsilon-61\right)C_A + \frac{1}{3}(\epsilon-1)(8\epsilon-7)C_F\right) iI_S^a\,, \end{aligned} \tag{28}$$

$$W_{\{1,2,0,2\}} = m^{-2\epsilon}\left(\frac{2(\epsilon-1)\left(2\epsilon^2-1\right)C_A}{2\epsilon-1} - \frac{4(\epsilon-1)\epsilon(2\epsilon+1)C_F}{2\epsilon-1} + \frac{1}{3}(1-\epsilon)n_h\right) iI_H$$
$$+\bar{\mu}^{-2\epsilon}\,\delta_1 Z_g + k^{-2\epsilon}\left(\frac{(\epsilon-1)n_l}{2\epsilon-3} - \frac{\left(40\epsilon^2-95\epsilon+51\right)C_A}{6(2\epsilon-3)}\right) iI_S^a\,, \tag{29}$$

$$W_{\{1,2,1,2\}} = k^{-2\epsilon}\left(\frac{1}{2}(\epsilon-2)C_A + \frac{1}{4}(-\epsilon-1)C_F\right) iI_S^b\,, \tag{30}$$

$$W_{\{1,2,3,0\}} = k^{-2\epsilon}\left(\frac{1}{8}\left(2\epsilon^2-6\epsilon+5\right)C_A + \frac{1}{16}\left(-6\epsilon^2+15\epsilon-14\right)C_F\right) iI_S^b\,, \tag{31}$$

$$W_{\{2,2,2,0\}} = m^{-2\epsilon}\left(\frac{1}{8}(1-\epsilon)C_A + \frac{(\epsilon-1)\epsilon C_F}{2(2\epsilon+1)}\right) iI_H - k^{-2\epsilon}\cdot\frac{1}{8}C_A iI_S^a\,, \tag{32}$$

$$W_{\{2,2,3,0\}} = -k^{-2\epsilon}\cdot\frac{\epsilon C_F}{16(\epsilon-1)}\, iI_S^b\,, \tag{33}$$

$$W_{\{4,2,0,0\}} = m^{-2\epsilon}\left(-\frac{(\epsilon-1)\left(2\epsilon^2-1\right)C_A}{2(2\epsilon-1)} + \frac{(\epsilon-1)\epsilon(2\epsilon+1)C_F}{2\epsilon-1} + \frac{1}{6}(\epsilon-1)n_h\right) iI_H$$
$$-\bar{\mu}^{-2\epsilon}\,\frac{\delta_1 Z_g}{2} + k^{-2\epsilon}\left(-\frac{(\epsilon-1)(4\epsilon-5)C_A}{4(2\epsilon-3)} - \frac{(\epsilon-1)n_l}{2(2\epsilon-3)}\right) iI_S^a\,, \tag{34}$$

$$W_{\{4,2,1,0\}} = k^{-2\epsilon}\left(\frac{\epsilon C_A}{8} - \frac{\left(2\epsilon^2-7\epsilon+4\right)C_F}{16(\epsilon-1)}\right) iI_S^b\,, \tag{35}$$

$$W_{\{5,2,0,0\}} = m^{-2\epsilon}\left(-\frac{(\epsilon-1)\left(2\epsilon^2-1\right)C_A}{2\epsilon-1} + \frac{2(\epsilon-1)\epsilon(2\epsilon+1)C_F}{2\epsilon-1} + \frac{1}{2}(\epsilon-1)n_h\right) iI_H$$
$$-\bar{\mu}^{-2\epsilon}\,\frac{3\delta_1 Z_g}{2} + k^{-2\epsilon}\left(-\frac{\left(24\epsilon^2-49\epsilon+21\right)C_A}{4(2\epsilon-3)} - \frac{3(\epsilon-1)n_l}{2(2\epsilon-3)}\right) iI_S^a\,, \tag{36}$$

$$W_{\{5,2,1,0\}} = k^{-2\epsilon}\left(\frac{1}{4}(3\epsilon-2)C_A + \frac{1}{4}(4-3\epsilon)C_F\right) iI_S^b\,. \tag{37}$$

The EBR master integrals of the hard and soft regions are given by

$$iI_H = (4\pi)^{\epsilon-2}\Gamma(\epsilon-1)\,,\quad iI_S^a = -\frac{2^{4\epsilon-5}\pi^{\epsilon-\frac{1}{2}}}{\sin(\pi\epsilon)\Gamma\left(\frac{3}{2}-\epsilon\right)}\,,\quad iI_S^b = \frac{16^{\epsilon-1}\pi^{\epsilon}}{\cos(\pi\epsilon)\Gamma(1-\epsilon)}\,, \tag{38}$$

(after factoring out the dimensionful parameters). The one-loop counter term for the gauge coupling constant reads

$$\delta_1 Z_g = \frac{2\left(n_h+n_l\right)-11C_A}{96\pi^2\epsilon}\,. \tag{39}$$

It is straightforward to expand the above Wilson coefficients in ϵ.

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