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Third-order non-Coulomb correction to the S-wave quarkonium wave functions at the origin

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Abstract

We compute the third-order correction to the S-wave quarkonium wave functions $|\psi_n(0)|^2$ at the origin from non-Coulomb potentials in the effective non-relativistic Lagrangian. Together with previous results on the Coulomb correction and the ultrasoft correction computed in a companion paper, this completes the third-order calculation up to a few unknown matching coefficients. Numerical estimates of the new correction for bottomonium and toponium are given.

1 Introduction

The non-relativistic bound-state problem has a long history since the birth of quantum mechanics. Its systematic derivation from the relativistic quantum field theory of electrodynamics or chromodynamics (QCD) was developed more recently. Non-relativistic effective field theories [1–3] together with dimensional regularization and diagrammatic expansion methods [4] now allow calculations of higher-order perturbative corrections, including all "relativistic" effects, to the leading-order bound-state properties, given by the solution of the Schrödinger equation. This is of interest in QCD for the lowest bottomonium state and top-antitop production near threshold, where non-perturbative long-distance effects can be argued to be sub-dominant, but perturbative corrections are large.

The S-wave energy levels are currently known at next-to-next-to-next-to-leading order (NNNLO) [5–8], except for the three-loop coefficient of the colour-Coulomb potential, but the corresponding wave functions at the origin, which are related to electromagnetic decay and production of these states are completely known only at next-to-next-to-leading order (NNLO) [9–11]. There exist partial results for logarithmic effects at NNNLO [12–15], which can be related to certain anomalous dimensions and lower-order quantities. In [7] we computed the third-order corrections to S-wave wave function at the origin from all terms in the heavy-quark potential related only to the Coulomb potential. In this paper we compute the contribution from the remaining potentials. A companion paper [16] deals with the Lamb-shift like contribution from ultrasoft gluons, thus completing the calculation of all bound-state effects at NNNLO, except for a few unknown matching coefficients. Our result is provided in such a form that these coefficients can be easily inserted, once they are computed.

In contrast to the Coulomb corrections the calculation of the more singular non-Coulomb potential corrections leads to divergences, both in the calculation of the potentials themselves as in the insertions of these potentials in the calculation of the wave function at the origin. We employ dimensional regularization with $d = 4-2\epsilon$ throughout, and provide a precise definition of all quantities, which corresponds to the $\overline{\mathrm{MS}}$ subtraction scheme. The technical details of this calculation together with an extension to the full S-wave Green function will be given elsewhere.

2 Relating the leptonic quarkonium decay constant to the wave function at the origin

We consider the two-point function

$$\left(q^\mu q^\nu - g^{\mu\nu} q^2\right) \Pi(q^2) = i \int d^d x \, e^{iqx} \, \langle \Omega | T(j^\mu(x) j^\nu(0)) | \Omega \rangle, \tag{1}$$

of the electromagnetic heavy-quark current $j^\mu = \bar{Q}\gamma^\mu Q$, choosing $q^\mu = (2m + E, \mathbf{0})$ with m the pole mass of the heavy quark. The two-point function exhibits the S-wave bound-state poles at E_n, near which

$$\Pi(q^2) \stackrel{E\to E_n}{=} \frac{N_c}{2m^2}\,\frac{Z_n}{E_n - E - i\epsilon}. \tag{2}$$

Here $N_c = 3$ denotes the number of colours. The residue Z_n is related to the leptonic decay width $\Gamma([Q\bar{Q}]_n \to l^+l^-)$ of the nth S-wave quarkonium state by

$$\Gamma([Q\bar{Q}]_n \to l^+l^-) = \frac{4\pi N_c e_Q^2 \alpha^2 Z_n}{3m^2}, \tag{3}$$

with e_Q the electric charge of the heavy quark in units of the positron charge, and α the fine-structure constant. Although there are no toponium states, and the cross section of top-antitop production is determined by the full two-point function, the residue Z_n for $n = 1$ provides an approximation to the height of the broad resonance in this cross section.

The electromagnetic current j^μ is expressed in terms of the non-relativistic heavy quark (ψ) and anti-quark (χ) field operators via

$$j^{\,i} = c_v\,\psi^\dagger\sigma^i\chi + \frac{d_v}{6m^2}\psi^\dagger\sigma^i\,\mathbf{D^2}\chi + \ldots, \tag{4}$$

where the hard matching coefficients have expansions $c_v = 1 + \sum_n c_v^{(n)}(\alpha_s/4\pi)^n$, and the $d_v = 1 + d_v^{(1)}(\alpha_s/4\pi) + \ldots$. The central quantity in this paper is the two-point function

$$\begin{aligned} G(E) &= \frac{i}{2N_c(d-1)}\int d^dx\, e^{iEx^0}\,\langle\Omega|T(\,[\psi^\dagger\sigma^i\chi](x)\,[\chi^\dagger\sigma^i\psi](0))|\Omega\rangle \\ &\stackrel{E\to E_n}{=} \frac{|\psi_n(0)|^2}{E_n - E - i\epsilon}, \end{aligned} \tag{5}$$

defined in non-relativistic QCD (NRQCD), whose poles define the wave functions at the origin and bound-state energy levels. At leading order, the wave functions and binding energies are given by $|\psi_n^{(0)}(0)|^2 = (mC_F\alpha_s)^3/(8\pi n^3)$ and $E_n^{(0)} = -m(\alpha_s C_F)^2/(4n^2)$, respectively (here and below $C_F = (N_c^2-1)/(2N_c) = 4/3, C_A = N_c = 3$). They receive perturbative corrections from higher-order heavy-quark potentials and dynamical gluon effects, hence $E_n = E_n^{(0)}\,(1+\sum_k(\alpha_s/4\pi)^k e_k)$ and $|\psi_n(0)|^2 = |\psi_n^{(0)}(0)|^2\,(1+\sum_k(\alpha_s/4\pi)^k f_k)$. Using an equation-of-motion relation, we can replace $\mathbf{D^2}$ in (4) by $-mE$, and we obtain

$$Z_n = c_v\left[c_v - \frac{E_n}{m}\left(1 + \frac{d_v}{3}\right) + \cdots\right]|\psi_n(0)|^2, \tag{6}$$

where terms beyond NNNLO are neglected. Inserting the perturbative expansions and defining $Z_n = |\psi_n^{(0)}(0)|^2\,(1 + \sum_k(\alpha_s/4\pi)^k z_k)$, results in

$$z_1 = 2c_v^{(1)} + f_1, \tag{7}$$

$$z_2 = 2c_v^{(2)} + {c_v^{(1)}}^2 + 2c_v^{(1)} f_1 + f_2 - \frac{4E_n^{(0)}}{3m}, \tag{8}$$

$$\begin{aligned} z_3 &= 2c_v^{(3)} + 2c_v^{(1)}\left(c_v^{(2)} + f_2\right) + \left(2c_v^{(2)} + {c_v^{(1)}}^2\right) f_1 + f_3 \\ &\quad - \frac{E_n^{(0)}}{m}\left[\frac{d_v^{(1)}}{3} + \frac{4}{3}\left(c_v^{(1)} + e_1 + f_1\right)\right]. \end{aligned} \tag{9}$$

Note that e_k, f_k and z_k depend on the principal quantum number n of the energy level, but we omitted a corresponding index to keep the notation short. The short-distance coefficients $c_v^{(1)}$, $c_v^{(2)}$ in the $\overline{\mathrm{MS}}$ scheme[1] are given in [17,18]. The third-order coefficient $c_v^{(3)}$ is not yet known except for the n_f terms (n_f is the number of quarks whose mass is set to zero) [19]. The one-loop correction to the derivative current can be obtained by applying a spin-triplet projection to the results given in [20], which gives

$$d_v^{(1)} = -C_F\left[32 \ln \frac{\mu}{m} + \frac{16}{3}\right]. \tag{10}$$

Here the infrared-divergent part $d_v^{(1,\mathrm{div})} = -16C_F/\epsilon$ is subtracted and added back to the ultrasoft calculation, where it cancels an ultraviolet divergence [16]. The first- and second-order corrections e_1, f_1 and f_2 are summarized in [7].[2] The key quantity in the present work is the third-order correction $f_3 = f_3^C + f_3^{nC} + f_3^{\mathrm{us}}$, which we split into three parts: f_3^C from the Coulomb potential given in [7] (see also [8]); f_3^{nC} accounting for all remaining potential insertions calculated below; and the ultrasoft correction $f_3^{\mathrm{us}} = 64\pi^2\delta^{us}\psi_n$ calculated in [16]. Note that e_1, f_1, $c_v^{(1)}$ are finite, but all other expansion coefficients $c_v^{(2)}$, $c_v^{(3)}$, $d_v^{(1)}$, f_2 and f_3^C, f_3^{nC}, f_3^{us} depend on a convention for regularizing (and subtracting) various ultraviolet and infrared divergences that arise in separating the contributions from the different scales. These divergences cancel in the expansion coefficients z_k, since Z_n is an observable. We regulate all ultraviolet (UV) as well as infrared (IR) divergences dimensionally, and adopt the $\overline{\mathrm{MS}}$ subtraction scheme, but we also check explicitly that the pole parts of the various terms cancel in the sums (9) wherever possible.

3 Potentials

Starting from full QCD, potentials arise after integrating out hard and soft modes, and potential gluons [21]. The potential NRQCD (PNRQCD) [2] effective Lagrangian contains a series of instantaneous interactions (potentials) with matching coefficients computed to an appropriate order in perturbation theory, and the interactions of ultrasoft

[1] The $\overline{\mathrm{MS}}$ scheme is defined by the loop integration measure $\tilde{\mu}^{2\epsilon} d^d k/(2\pi)^d$ with $\tilde{\mu}^2 = \mu^2\, e^{\gamma_E}/(4\pi)$ and subtraction of the pole parts in ϵ.

[2] In Eq. (30) of the published version of [7], the term $-E_n^{(0)}/m$ in (8) that comes from the expansion of q^2 around $4m^2$ was incorrectly included in the formula for f_2^{nC}. The term $-13/(8n^2)$ in Eq. (30) should therefore read $-15/(8n^2)$. This is corrected in [hep-ph/0501289v2].

gluons. In this paper we do not consider the ultrasoft gluon interactions (see [16]), so the required Lagrangian is

$$\mathcal{L} = \psi^\dagger\Big(i\partial_0 + \frac{\boldsymbol{\partial}^2}{2m} + \frac{\boldsymbol{\partial}^4}{8m^3}\Big)\psi + \chi^\dagger\Big(i\partial_0 - \frac{\boldsymbol{\partial}^2}{2m} - \frac{\boldsymbol{\partial}^4}{8m^3}\Big)\chi \\ + \int d^{d-1}\mathbf{r}\,\Big[\psi^\dagger\psi\Big](x+\mathbf{r})\,\Big(V_0(r) + \delta V(r,\boldsymbol{\partial})\Big)\,\Big[\chi^\dagger\chi\Big](x). \tag{11}$$

In the first line relativistic corrections to the kinetic energy are included; the second line shows the potentials with δV the correction to the leading-order Coulomb potential V_0. The general form of the potential is colour- and spin-dependent. In writing (11) we have made simplifications that apply to the computation of the Green function of colour-singlet, spin-triplet currents. We have also used that annihilation diagrams contribute to this Green function only from the fourth order. Since we work in dimensional regularization, the spin-triplet projection has to be carried out consistently in d dimensions, which implies $\mathrm{tr}(\sigma^i\sigma^i) = 2(d-1)$ for the Pauli matrices. Furthermore one must not use the ϵ-symbol, and treat the commutator $[\sigma^i,\sigma^j]$ as irreducible. For the calculation the momentum space representation of δV is more convenient. It can be written in the form ($\mathbf{q} = \mathbf{p} - \mathbf{p}'$)

$$\delta\widetilde{V} = -\frac{4\pi\alpha_s C_F}{\mathbf{q}^2}\Big[\mathcal{V}_C - \mathcal{V}_{1/m}\frac{\pi^2\,|\mathbf{q}|}{m} + \mathcal{V}_{1/m^2}\frac{\mathbf{q}^2}{m^2} + \mathcal{V}_p\frac{\mathbf{p}^2 + \mathbf{p}'^2}{2m^2}\Big]. \tag{12}$$

The strong coupling constant $\alpha_s = \alpha_s(\mu)$ is renormalized at the scale μ unless stated otherwise. The coefficients $\mathcal{V}_i$ can be expanded in α_s,

$$\mathcal{V}_i = \mathcal{V}_i^{(0)} + \frac{\alpha_s}{4\pi}\mathcal{V}_i^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2\mathcal{V}_i^{(2)} + \mathcal{O}(\alpha_s^3), \tag{13}$$

with the superscript denoting the number of loops. The tree-level Coulomb potential $\mathcal{V}_C^{(0)}$ is a leading effect and is therefore included in $V_0(r)$ in the Lagrangian. For the calculation of the third-order non-Coulomb correction we need $\mathcal{V}_{1/m}$ to two loops, and $\mathcal{V}_{1/m^2}$, $\mathcal{V}_p$ to one loop. We also need the one-loop Coulomb potential to calculate the double insertion of $\mathcal{V}_C^{(1)}$ with $\mathcal{V}_{1/m^2}^{(0)}$ and $\mathcal{V}_p^{(0)}$.

The potentials must be determined in d dimensions, since the subsequent insertions are ultraviolet divergent. We now summarize the expansion coefficients. The tree-level coefficients are [11]

$$\mathcal{V}_p^{(0)} = 1, \quad \mathcal{V}_{1/m}^{(0)} = 0, \quad \mathcal{V}_{1/m^2}^{(0)} \equiv v_0(\epsilon) = -\frac{4-\epsilon-2\epsilon^2}{6-4\epsilon}. \tag{14}$$

The matching coefficients in PNRQCD receive contributions from hard momenta $k \sim m$ and soft momenta $\mathbf{k} \sim m\alpha_s$. Including counterterms (see below) the d-dimensional coefficients assume the form ($\beta_0 = 11C_A/3 - 4T_F n_f/3$)

$$\mathcal{V}_C^{(1)} = \left[\left(\frac{\mu^2}{\mathbf{q}^2}\right)^\epsilon - 1\right]\frac{\beta_0}{\epsilon} + \left(\frac{\mu^2}{\mathbf{q}^2}\right)^\epsilon a_1(\epsilon), \tag{15}$$

$$\mathcal{V}^{(1)}_{1/m} = \left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon} b_1(\epsilon), \tag{16}$$

$$\begin{aligned}\mathcal{V}^{(2)}_{1/m} &= \left[\left(\frac{\mu^2}{\mathbf{q^2}}\right)^{2\epsilon} - 1\right] \left(-\frac{8}{3\epsilon}\right)\left(2C_FC_A + C_A^2\right) \\ &\quad + \left[\left(\frac{\mu^2}{\mathbf{q^2}}\right)^{2\epsilon} - \left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon}\right] \frac{2\beta_0}{\epsilon}\, b_1(\epsilon) + \left(\frac{\mu^2}{\mathbf{q^2}}\right)^{2\epsilon} 4b_2(\epsilon),\end{aligned} \tag{17}$$

$$\begin{aligned}\mathcal{V}^{(1)}_{1/m^2} &= \left[\left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon} - 1\right] \frac{1}{\epsilon}\left(\frac{7}{3}C_F - \frac{11}{6}C_A + \beta_0\, v_0(\epsilon)\right) \\ &\quad + \left[\left(\frac{\mu^2}{m^2}\right)^{\epsilon} - 1\right] \frac{1}{\epsilon}\left(\frac{C_F}{3} + \frac{C_A}{2}\right) + \left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon} v_q^{(1)}(\epsilon) + \left(\frac{\mu^2}{m^2}\right)^{\epsilon} v_m^{(1)}(\epsilon),\end{aligned} \tag{18}$$

$$\mathcal{V}^{(1)}_{p} = \left[\left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon} - 1\right] \frac{1}{\epsilon}\left(\frac{8}{3}C_A + \beta_0\right) + \left(\frac{\mu^2}{\mathbf{q^2}}\right)^{\epsilon} v_p^{(1)}(\epsilon). \tag{19}$$

The calculation of the coefficients $\mathcal{V}^{(2)}_{1/m}$, $\mathcal{V}^{(1)}_{1/m^2}$ and $\mathcal{V}^{(1)}_{p}$ results in IR divergences [22]. In writing the above equations, we subtracted the expression

$$\begin{aligned}\delta\widetilde{V}_{c.t.} &= \frac{\alpha_s C_F}{6\epsilon}\Bigg[C_A^3\frac{\alpha_s^3}{\mathbf{q}^2} + 4\left(C_A^2 + 2C_AC_F\right)\frac{\pi\alpha_s^2}{m|\mathbf{q}|} \\ &\quad + 16\left(C_F - \frac{C_A}{2}\right)\frac{\alpha_s}{m^2} + 16C_A\frac{\alpha_s}{m^2}\frac{(\mathbf{p^2}+\mathbf{p'^2})}{2\mathbf{q^2}}\Bigg],\end{aligned} \tag{20}$$

which corresponds to a $\overline{\mathrm{MS}}$ definition of the spin-projected potentials as PNRQCD matching coefficients. The counterterm (20) is added back to the ultrasoft contribution [16], where it cancels a corresponding UV divergence. The terms proportional to β_0/ϵ in (15) to (19) are related to QCD charge renormalization. With the exception of $b_1(\epsilon)$, which we need to second order in the ϵ-expansion, all other coefficients are needed at the first order. Their expressions are

$$a_1(\epsilon) = \left(C_A\,[11-8\epsilon] - 4\,T_Fn_f\right)\frac{e^{\epsilon\gamma_E}\,\Gamma(1-\epsilon)\,\Gamma(2-\epsilon)\,\Gamma(\epsilon)}{(3-2\,\epsilon)\,\Gamma(2-2\,\epsilon)} - \frac{\beta_0}{\epsilon}, \tag{21}$$

$$b_1(\epsilon) = \left(\frac{C_F}{2}\,[1-2\epsilon] - C_A\,[1-\epsilon]\right)\frac{e^{\epsilon\gamma_E}\,\Gamma(\frac{1}{2}-\epsilon)^2\Gamma(\frac{1}{2}+\epsilon)}{\pi^{\frac{3}{2}}\,\Gamma(1-2\epsilon)}, \tag{22}$$

$$\begin{aligned}b_2(\epsilon) &= \left[\frac{65}{18} - \frac{8}{3}\ln 2\right]C_AC_F - \left[\frac{101}{36} + \frac{4}{3}\ln 2\right]C_A^2 \\ &\quad + \left[\frac{49}{36}\,C_A - \frac{2}{9}C_F\right]T_Fn_f + \epsilon\, b_2^{(\epsilon)},\end{aligned} \tag{23}$$

$$v_q^{(1)}(\epsilon) = -\frac{C_F}{3} - \frac{11}{27}C_A + \frac{40}{27}\,T_Fn_f + \epsilon\, v_q^{(1,\epsilon)}\,, \tag{24}$$

$$v_m^{(1)}(\epsilon) = -\frac{C_F}{3} - \frac{29}{9}C_A + \frac{4}{15}T_F + \epsilon\, v_m^{(1,\epsilon)}\,, \tag{25}$$

$$v_p^{(1)}(\epsilon) = \frac{31}{9}C_A - \frac{20}{9}T_F n_f + \epsilon\, v_p^{(1,\epsilon)}, \tag{26}$$

where we checked the d-dimensional expression for $a_1(\epsilon)$ in [23], $b_1(\epsilon)$ is from [11], $b_2(\epsilon = 0)$ from [24], and $v_i^{(1)}(\epsilon = 0)$ for $i = \{q, m, p\}$ are obtained from [6,25][3]. The $O(\epsilon)$ term of $b_2(\epsilon)$ is unknown; the corresponding terms $v_i^{(1,\epsilon)}$ can be obtained from [25]. However, in the present work, we shall use this result only for a rough estimate.

4 Third-order non-Coulomb correction to the wave function at the origin

Since the relevant terms in the effective Lagrangian (11) do not take us out of the quark-antiquark sector of the Fock space, the calculation of $G(E)$ can be mapped to a Hamiltonian problem in single-particle quantum mechanics after separating the trivial center-of-mass motion of the quark-antiquark pair. At leading order $G(E)$ equals the Green function

$$G_0(E) \equiv \langle 0|\hat{G}_0|0\rangle = \langle 0|\frac{1}{H_0 - E - i\epsilon}|0\rangle, \tag{27}$$

of the Schrödinger operator $H_0 = \boldsymbol{\nabla}^2/m - \alpha_s C_F/r$ with $|0\rangle$ denoting a relative position eigenstate with eigenvalue $\mathbf{r} = 0$. The effect of the perturbation potentials δV is taken into account by substituting $H_0 \to H = H_0 + \delta V$, and then the Green function $G(E)$ is systematically expanded in powers of α_s. The third-order non-Coulomb correction corresponds to the expression

$$\delta_3 G = 2\,\langle 0|\hat{G}_0\delta V_1\hat{G}_0\delta V_2\hat{G}_0|0\rangle - \langle 0|\hat{G}_0\delta V_3\hat{G}_0|0\rangle \tag{28}$$

with δV_1 the one-loop Coulomb potential contribution to δV, and δV_2, δV_3 the second and third order non-Coulomb potentials in momentum space given by

$$\delta\widetilde{V}_2 = -\frac{\mathbf{p}^4}{4m^3}\,\delta^{(d-1)}(\mathbf{p}-\mathbf{p}') + \delta\widetilde{V}_{1/m}^{(1)} + \delta\widetilde{V}_{1/m^2}^{(0)} + \delta\widetilde{V}_p^{(0)}, \tag{29}$$

$$\delta\widetilde{V}_3 = \delta\widetilde{V}_{1/m}^{(2)} + \delta\widetilde{V}_{1/m^2}^{(1)} + \delta\widetilde{V}_p^{(1)}, \tag{30}$$

where the first term in $\delta\widetilde{V}_2$ is due to the relativistic kinetic energy correction in (11), and $\delta\widetilde{V}_X^{(k)}$ refers to the corresponding terms in (15) to (19) including the prefactors in (12). The result of the potential insertions (28) is matched to the pole structure of $G(E)$, which allows us to extract the bound-state energy and its wave function at the

[3]The coefficient $v_p^{(1)}$ corresponds to $-d_1^p$ in [6].

origin. The technical details of the calculation will be discussed elsewhere. Here we briefly summarize the main results.

The expression (28) should be considered as an infinite sum of loop diagrams defined in dimensional regularization. Since the $(d-1)$-dimensional Coulomb Green function $\hat{G}_0$ is not known in closed form, one must separate the divergent subgraphs. Since these contain only a finite number of loops and since the divergent part is local, one calculates these subgraphs in d dimensions and factorizes the pole part from the remainder of the diagram. All non-divergent diagrams can be computed in $d=4$ using the known three-dimensional Coulomb Green function. For the divergent part of (28) we find

$$\begin{aligned}
\delta_3 G_{div} = \Bigg[& -\frac{1}{\epsilon^2}\left(\frac{7}{72}C_F^2 + \frac{2}{9}C_A^2 + \frac{23}{48}C_A C_F + \beta_0\left(\frac{C_A}{24}+\frac{C_F}{36}\right)\right) \\
& -\frac{1}{\epsilon}\Bigg\{\left(\frac{11}{24}-\frac{L_m}{12}\right)C_F^2 + \left(\frac{427}{324}-\frac{4\ln 2}{3}-\frac{L_m}{8}\right)C_A C_F - \left(\frac{5}{216}+\frac{2\ln 2}{3}\right)C_A^2 \\
& +\left(\frac{C_A}{24}+\frac{C_F}{54}\right)\beta_0 - \left(\frac{1}{30}-\frac{29\,n_f}{162}\right)C_F T_F + \frac{49}{216}C_A T_F n_f\Bigg\}\Bigg]\,\frac{\alpha_s^3 C_F}{\pi}\,\langle 0|\hat{G}_0|0\rangle \\
& -\left[\frac{1}{4}C_A + \frac{1}{6}C_F\right]\frac{\alpha_s^2 C_F}{\epsilon}\,\langle 0|\hat{G}_0\delta V_1\hat{G}_0|0\rangle
\end{aligned} \tag{31}$$

with $L_m = \ln(\mu/m)$. In the residue Z_n the pole part in the last line cancels against a corresponding term in the contribution $2c_v^{(2)}f_1$ in (9), while the divergent part proportional to $G_0(E)$ combines with similar terms in the ultrasoft contribution, and must cancel with $2c_v^{(3)}$. From the finite part of $\delta_3 G$, we extract the non-Coulomb contribution to f_3, and obtain

$$\begin{aligned}
\frac{f_3^{nC}}{64\pi^2} = & \left[\frac{7}{6}C_F^3 + \frac{37}{12}C_A C_F^2 + \frac{4}{3}C_A^2 C_F + \beta_0\left(\frac{4}{3}C_F^2 + 2C_A C_F\right)\right]L^2 \\
& + \Bigg[C_F^3\left(-\frac{3}{2}+\frac{14}{3n}-\frac{7S_1}{3}\right) + C_A C_F^2\left(\frac{226}{27}+\frac{8\ln 2}{3}+\frac{37}{3n}-\frac{5}{3n^2}-\frac{37S_1}{6}\right) \\
& + C_A^2 C_F\left(\frac{145}{18}+\frac{4\ln 2}{3}+\frac{16}{3n}-\frac{8S_1}{3}\right) + C_F^2\,T_F\left(\frac{2}{15}-\frac{59}{27}n_f\right) \\
& - \frac{109}{36}C_A C_F T_F\,n_f + \beta_0\Bigg\{C_F^2\left(\frac{16}{3}+\frac{10}{3n}-\frac{75}{16n^2}-\frac{\pi^2 n}{9}-\frac{4S_1}{3}+\frac{2nS_2}{3}\right) \\
& + C_A C_F\left(\frac{15}{8}+\frac{5}{n}-\frac{\pi^2 n}{6}-2S_1+nS_2\right)\Bigg\}\Bigg]L + \left[\frac{1}{3}C_F^3 + \frac{1}{2}C_A C_F^2\right]L_m L \\
& + \left[\frac{1}{12}C_F^3 + \frac{1}{8}C_A C_F^2\right]L_m^2 + \Bigg[C_F^3\left(\frac{1}{12}+\frac{2}{3n}-\frac{S_1}{3}\right) + C_A C_F^2\left(-\frac{5}{9}+\frac{1}{n}-\frac{S_1}{2}\right) \\
& + \frac{1}{15}C_F^2 T_F\Bigg]L_m + \frac{c_{\psi,3}^{nC}}{64\pi^2},
\end{aligned} \tag{32}$$

where $L \equiv \ln(n\mu/(m\, C_F\, \alpha_s))$, and the unwritten argument n of the harmonic sum $S_a = S_a(n) \equiv \sum_{k=1}^{n} 1/k^a$ is the principle quantum number n. The non-logarithmic part[4] is given by

$$
\begin{aligned}
\frac{c_{\psi,3}^{nC}}{64\pi^2} = & \left[-\frac{137}{36} - \frac{49\pi^2}{432} - \frac{25}{6n} + \frac{35}{12n^2} + S_1\left(\frac{3}{2} - \frac{14}{3n} + \frac{7S_1}{6}\right) - \frac{7S_2}{6}\right] C_F^3 \\
& + \left[\frac{7061}{486} - \frac{50\pi^2}{81} + \frac{1475}{108n} + \frac{\pi^2}{9n} - \frac{321}{32n^2} + \ln 2\left(\frac{353}{54} + \frac{16}{3n} - \frac{16\ln 2}{9}\right) \right. \\
& \qquad \left. - S_1\left(\frac{226}{27} + \frac{8\ln 2}{3} + \frac{37}{3n} + \frac{1}{n^2} - \frac{37S_1}{12}\right) - S_2\left(\frac{37}{12} + \frac{2}{3n}\right)\right] C_A C_F^2 \\
& + \left[\frac{3407}{432} - \frac{5\pi^2}{18} + \frac{133}{9n} + \ln 2\left(\frac{187}{108} + \frac{8}{3n} - \frac{8\ln 2}{9}\right) - \frac{4S_2}{3} \right. \\
& \qquad \left. - S_1\left(\frac{145}{18} + \frac{4\ln 2}{3} + \frac{16}{3n} - \frac{4S_1}{3}\right)\right] C_A^2 C_F + \left[\frac{1}{15} + \frac{4}{15n} - \frac{2S_1}{15}\right] C_F^2 T_F \\
& + \left[-\frac{361}{108} + \frac{49\ln 2}{108} - \frac{109}{18n} + \frac{109S_1}{36}\right] C_A C_F T_F\, n_f \\
& + \left[-\frac{3391}{486} + \frac{5\pi^2}{648} - \frac{2\ln 2}{27} - \frac{118}{27n} + \frac{125}{24n^2} + \frac{59S_1}{27}\right] C_F^2 T_F\, n_f \\
& + \beta_0 \left[\left\{ \frac{1027}{648} + \frac{19}{6n} + \frac{25}{24n^2} - \frac{35\pi^2}{108} - \frac{11\pi^2 n}{27} + \frac{5\pi^2}{16n} + \frac{4nS_3}{3} - \frac{2nS_{2,1}}{3} \right.\right. \\
& \qquad \left. - S_1\left(\frac{10}{9} + \frac{1}{3n} + \frac{45}{16n^2} - \frac{\pi^2 n}{9} + \frac{2nS_2}{3}\right) + S_2\left(1 + \frac{22n}{9} - \frac{15}{8n}\right)\right\} C_F^2 \\
& \qquad + \left\{ \frac{7}{24} - \frac{91\pi^2}{144} - \frac{1}{4n} - \frac{5\pi^2 n}{24} - S_1\left(\frac{3}{8} + \frac{1}{2n} - \frac{\pi^2 n}{6} + nS_2\right) + S_2\left(\frac{3}{2} + \frac{5n}{4}\right) \right. \\
& \qquad \left.\left. - nS_{2,1} + 2nS_3 \right\} C_A C_F \right] + \delta_\epsilon, \qquad (33)
\end{aligned}
$$

where $S_{a,b} = S_{a,b}(n) \equiv \sum_{k=1}^{n} S_b(k)/k^a$ is a nested harmonic sum, and

$$
\delta_\epsilon = \left(\frac{v_m^{(1,\epsilon)}}{8} + \frac{v_q^{(1,\epsilon)}}{12} + \frac{v_p^{(1,\epsilon)}}{12}\right) C_F^2 - \frac{C_F}{6}\, b_2^{(\epsilon)}, \qquad (34)
$$

denotes the contribution from the unknown $O(\epsilon)$ terms of the potentials. Note that δ_ϵ is independent of the principal quantum number n.

[4]For some of the terms in our calculation, we obtained analytic expressions which can be evaluated only for any given value of n. To obtain the presented result for general n, we made a rather general ansatz for the possible dependence on n such as harmonic sums and determined the rational coefficients of the various structures from the analytic result for $n = 1, 2, \ldots, 8$. The correctness of this result was then checked for all further n up to $n = 30$.

5 Numerical results

We briefly discuss the numerical significance of the non-Coulomb correction. The numbers below should be considered as indicating the typical size of the correction. The correction itself is strongly scale-dependent and a physically relevant result is only obtained by combining all terms in (9). This cannot be done, since $c_v^{(3)}$ and δ_ϵ are still unknown.

The numerical expressions of the non-Coulomb wave function correction to the lowest three states $n = 1, 2, 3$ are given by $(\delta_3|\psi_n(0)|^2_{nC} = |\psi_n^{(0)}(0)|^2(\alpha_s/(4\pi))^3 f_3^{nC})$

$$\delta_3|\psi_1(0)|^2_{nC} = \frac{(m\alpha_s C_F)^3}{8\pi}\,\frac{\alpha_s^3}{\pi}\Big[(149.3 - 6.9n_f)\,L^2 + 0.9L_m^2 + 3.5L\,L_m + (449.8 - 21.9n_f)\,L + 0.8L_m + (-149.7 - 3.1n_f) + \delta_\epsilon\Big], \tag{35}$$

$$\delta_3|\psi_2(0)|^2_{nC} = \frac{(m\alpha_s C_F)^3}{64\pi}\,\frac{\alpha_s^3}{\pi}\Big[(149.3 - 6.9n_f)\,L^2 + 0.9L_m^2 + 3.5L\,L_m + (211.7 - 13.5n_f)\,L - 4.4L_m + (-217.9 + 2.7n_f) + \delta_\epsilon\Big], \tag{36}$$

$$\delta_3|\psi_3(0)|^2_{nC} = \frac{(m\alpha_s C_F)^3}{216\pi}\,\frac{\alpha_s^3}{\pi}\Big[(149.3 - 6.9n_f)\,L^2 + 0.9L_m^2 + 3.5L\,L_m + (89.7 - 8.8n_f)\,L - 6.7L_m + (-218.3 + 5.1n_f) + \delta_\epsilon\Big], \tag{37}$$

Since some of the $O(\epsilon)$ parts of the potentials, δ_ϵ, are not known, we perform a crude estimate. We derive the expressions for $v_i^{(1,\epsilon)}$, $i = m, q, p$ from [25], and estimate $b_2^{(\epsilon)}/b_2(\epsilon = 0)$ by the corresponding ratio for $b_1(\epsilon)$, allowing for a factor ± 2 variation in this ratio. In this way our estimate, $\delta_\epsilon \approx (-3 \ldots + 8)$, is dominated by $b_2^{(\epsilon)}$, but is more than an order of magnitude smaller than the other non-logarithmic terms. Below, we therefore set δ_ϵ to zero. The potential scale is of order $m\alpha_s C_F$, while the natural choice for the hard factorization scale is m. In the following we show the size of the non-Coulomb correction for two scale choices, $\mu_B = mC_F\alpha_s(\mu_B)$ and $\mu = m$.

"Toponium" wave function at the origin. For the top-antitop production cross section near threshold, the height of the smeared resonance is related to the wave function at the origin of the $n = 1$ ground state. The two scales discussed above correspond to $\alpha_s^{(n_f=5)}(\mu_B) = 0.140$ ($\mu_B = 32.6\,\mathrm{GeV}$) and $\alpha_s^{(n_f=5)}(m_t) = 0.107$ ($m_t = 175\,\mathrm{GeV}$). From (35), we obtain

$$\frac{\delta_3|\psi_1(0)|^2_{nC}}{|\psi_1^{(0)}(0)|^2} = \frac{\alpha_s^3(\mu_B)}{\pi}\Big(-165.1 + 0.8\,\ln(\alpha_s C_F) + 0.9\,\ln^2(\alpha_s C_F)\Big) = -0.14, \tag{38}$$

$$\frac{\delta_3|\psi_1(0)|^2_{nC}}{|\psi_1^{(0)}(0)|^2} = \frac{\alpha_s^3(m_t)}{\pi}\left(-165.1 + 340.3\ln\left(\frac{1}{\alpha_s C_F}\right) + 114.7\ln^2\left(\frac{1}{\alpha_s C_F}\right)\right) = 0.36, \tag{39}$$

where $\mu = \mu_B$ ($\mu = m_t$) is used in the first (second) line. Our estimate for δ_ϵ affects these numbers by less than 0.01. For comparison, the NNNLO Coulomb correction is $\delta_3|\psi_1(0)|^2_C/|\psi_1^{(0)}(0)|^2 = -0.04$ with $\mu = \nu = \mu_B$ (see [7]). The result above indicates a potentially very large third-order contribution from the non-Coulomb potentials. A similar observation is made for the ultrasoft contribution [16], and since the non-logarithmic terms of the non-Coulomb and ultrasoft contribution have opposite sign, a cancellation is possible.

Bottomonium. Here the QCD corrections to the wave function at the origin are known to be rather large, and the application of the perturbative calculation is certainly questionable for excited states [7]. Therefore, mainly the bottomonium ground state $\Upsilon(1S)$ is of phenomenological interest. The bound-state scale corresponds to $\alpha_s^{(n_f=4)}(\mu_B) = 0.30$ ($\mu_B = 2\,\mathrm{GeV}$), and the hard scale to $\alpha_s^{(n_f=4)}(5\,\mathrm{GeV}) = 0.21$ ($m_b = 5\,\mathrm{GeV}$). The non-Coulomb correction to the $\Upsilon(1S)$ wave function at the origin is

$$\frac{\delta_3|\psi_1(0)|^2_{nC}}{|\psi_1^{(0)}(0)|^2} = \frac{\alpha_s^3(\mu_B)}{\pi}\Big(-162.0 + 0.8\,\ln(\alpha_s C_F) + 0.9\,\ln^2(\alpha_s C_F)\Big) = -1.4, \tag{40}$$

$$\frac{\delta_3|\psi_1(0)|^2_{nC}}{|\psi_1^{(0)}(0)|^2} = \frac{\alpha_s^3(m_b)}{\pi}\left(-162.0 + 362.2\ln\Big(\frac{1}{\alpha_s C_F}\Big) + 121.6\ln^2\Big(\frac{1}{\alpha_s C_F}\Big)\right) = 1.5. \tag{41}$$

Once again, the contribution of δ_ϵ does not seem to be important. For comparison, the NNNLO Coulomb correction is $\delta_3|\psi_1(0)|^2_C/|\psi_1^{(0)}(0)|^2 = -0.47$ for $\mu = \mu_B$. In view of the size of this third-order correction the validity of a perturbative treatment of the leptonic $\Upsilon(1S)$ width relies on cancellations that might occur in the complete third-order correction.

6 Summary

We computed the third-order correction to the S-wave quarkonium wave functions at the origin originating from insertions involving potentials other than the Coulomb potential. The UV as well as IR divergences are regulated dimensionally in a way that is consistent with other parts of the calculation, performed in the context of the diagrammatic threshold expansion. Together with the previous calculation of the Coulomb potential contributions [7,8] and the ultrasoft contribution [16] this completes the bound-state part of the third-order calculation. The remaining unknowns are related to the finite parts of three-loop matching coefficients (a_3, $c_v^{(3)}$) and the $O(\epsilon)$ parts of one- and two-loop coefficients (parameterized here by δ_ϵ). Numerical estimates of the new non-Coulomb contribution suggest important third-order effects even for top quarks, but a definitive conclusion can only be drawn once the missing matching coefficients are computed.

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