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Heavy Quarkonium Spectrum and Production/Annihilation Rates to order $\beta_0^3\alpha_s^3$

A.A. Penin[a,b], V.A. Smirnov[c,d], M. Steinhauser[a]

[a] *Institut für Theoretische Teilchenphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany*

[b] *Institute for Nuclear Research, Russian Academy of Sciences, 117312 Moscow, Russia*

[c] *Institute for Nuclear Physics, Moscow State University, 119992 Moscow, Russia*

[d] *II. Institut für Theoretische Physik, Universität Hamburg, 22761 Hamburg, Germany*

Abstract

We compute the third-order corrections to the heavy quarkonium spectrum and production/annihilation rates due to the leading renormalization group running of the static potential. The previously known complete $\mathcal{O}(m_q\alpha_s^5)$ result for the heavy quarkonium ground state energy is extended to the exited states. After including the $\mathcal{O}(\alpha_s^3)$ corrections the perturbative results are in surprisingly good agreement with the experimental data on the masses of the excited Υ resonances and the leptonic width of the $\Upsilon(1S)$ meson. The impact of the corrections on the Υ sum rules and top quark-antiquark threshold production cross section is also discussed.

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1 Introduction

The theoretical study of nonrelativistic heavy quark-antiquark systems is among the earliest applications of perturbative quantum chromodynamics (QCD) [1]. Its applications to bottomonium [2] and top-antitop [3] physics entirely rely on the first principles of QCD. In general perturbation theory can be applied for the analysis of these systems. Nonperturbative effects [4,5] are well under control for the top-antitop system and, at least within the sum-rule approach, also for bottomonium. This makes heavy quark-antiquark systems an ideal laboratory to determine fundamental parameters of QCD, such as the strong coupling constant α_s and the heavy-quark masses m_q.

The binding energy of the heavy quarkonium state and the value of its wave function at the origin are among the characteristics of the heavy-quarkonium system that are of primary phenomenological interest. The former determines the mass of the bound state resonance, while the latter controls its production and annihilation rates.

Recently, the heavy quarkonium ground state energy has been computed through $\mathcal{O}(\alpha_s^5 m_q)$ including the third-order correction to the Coulomb approximation [6]. The result has been used to extract m_b from the $\Upsilon(1S)$ meson mass. The properties of the excited states are more sensitive to the nonperturbative phenomena, and the corresponding perturbative estimates cannot be used, *e.g.*, for the accurate determination of the heavy-quark mass by direct comparison to the meson masses. However, they have to be taken into account in the framework of the nonrelativistic sum rules [2] which is based on the concept of quark-hadron duality and keeps the nonperturbative effects under control. Moreover, by investigating the excited states with reliable perturbative results at hand one can test the effects and structure of the nonperturbative QCD vacuum. Still only a few states with small principal quantum numbers n and zero orbital momentum l are of practical interest.

As far as the wave function at the origin is concerned a complete result is only available through $\mathcal{O}(\alpha_s^2)$ [7,8]. The $\mathcal{O}(\alpha_s^2)$ correction has turned out to be so sizeable that the feasibility of an accurate perturbative analysis was challenged [9], and it appears indispensable to gain full control over the next order. Only the logarithmically enhanced $\mathcal{O}(\alpha_s^3 \ln^2 \alpha_s)$ [10,11] and $\mathcal{O}(\alpha_s^3 \ln \alpha_s)$ [12,13] (for QED, see Refs. [14–16]) corrections are available so far.

In this paper, we take the next step and calculate the nonlogarithmic third-order corrections to the wave function at the origin and to the spectrum of the excited heavy quarkonium states proportional to β_0^3, where β_0 is the one-loop QCD beta-function. Together with the contributions already known, the new term allows to derive the complete result for the binding energy of the excited states. On the other hand the large-β_0 terms usually constitute a considerable part of the corrections and can be used to estimate the unknown nonlogarithmic third-order contribution to the wave function.

In the next section we present the $\mathcal{O}(\beta_0^3 \alpha_s^3)$ corrections for the states with principle quantum number $n = 1,\ 2,\ 3$ and angular momentum $l = 0$. In Section 3 we generalize the complete $\mathcal{O}(m_q \alpha_s^5)$ result for the ground state energy [6] to the excited states. In Section 4 we discuss the impact of the corrections on the phenomenology of the $b\bar{b}$ and $t\bar{t}$

systems. Our summary is presented in Section 5.

2 Heavy quarkonium parameters to $\mathcal{O}(\beta_0^3\alpha_s^3)$

In the framework of nonrelativistic effective theory [17–20] the corrections to the heavy quarkonium parameters are obtained by evaluating the corrections to the Green function of the effective Schrödinger equation [21]. The β_0^3 part of the third-order contribution results from the leading renormalization group running of the static potential which enters the corresponding effective Hamiltonian and is given by (see also Ref. [22])

$$\begin{aligned} V_C(r) &= -\frac{C_F\alpha_s}{r}\Bigg\{1+\frac{\alpha_s}{4\pi}\left(8\beta_0 L_r+a_1\right)+\left(\frac{\alpha_s}{4\pi}\right)^2\Bigg[64\beta_0^2L_r^2+\left(16a_1\beta_0+32\beta_1\right)L_r \\ &\quad +a_2+\frac{16\pi^2}{3}\beta_0^2\Bigg]+\left(\frac{\alpha_s}{4\pi}\right)^3\Bigg[512\beta_0^3L_r^3+\left(192a_1\beta_0^2+640\beta_0\beta_1\right)L_r^2 \\ &\quad +\left(128\pi^2\beta_0^3+24a_2\beta_0+64a_1\beta_1+128\beta_2+16\pi^2C_A^3\right)L_r \\ &\quad +a_3+16\pi^2a_1\beta_0^2+1024\zeta(3)\beta_0^3+\frac{160\pi^2}{3}\beta_0\beta_1\Bigg]+\mathcal{O}(\alpha_s^4)\Bigg\}, \end{aligned} \tag{1}$$

where $L_r=\ln(e^{\gamma_E}\mu r)$, $\gamma_E=0.577216\ldots$ is Euler's constant, $\zeta(z)$ is Riemann's zeta-function with value $\zeta(3)=1.202057\ldots$, $C_F=(N_c^2-1)/(2N_c)$ and $C_A=N_c$ for the $SU(N_c)$ gauge group. Furthermore, we have $\alpha_s\equiv\alpha_s(\mu)$ if not stated otherwise. The coefficients a_i $(i=1,2)$ and β_i $(i=0,1,2)$ are given in Appendix A. For the three-loop coefficient a_3 only Padé estimates are available so far [23]. In the order of interest one has to consider single iterations of the β_0^3 term, double iterations of the β_0^2 and β_0 term and triple iterations of the first-order corrections proportional to β_0. For the practical computation we use the method elaborated in Refs. [24,7,25]. In this way we obtain the corrections to the energy levels and wave function at the origin in the form of multiple harmonic sums. For general n the result is rather cumbersome. For a specific n, however, the summation can be performed analytically. Below we present our result for $n=1,\ 2,\ 3$ and $l=0$ which is sufficient for the phenomenological applications. For vanishing angular momentum we can write the perturbative part of the energy level with principal quantum number n as

$$E_n^{\text{p.t.}} = E_n^C+\delta E_n^{(1)}+\delta E_n^{(2)}+\delta E_n^{(3)}+\ldots, \tag{2}$$

where $\delta E_n^{(k)}$ stands for corrections of order α_s^k. The leading order Coulomb energy is given by

$$E_n^C = -\frac{C_F^2\alpha_s^2 m_q}{4n^2}. \tag{3}$$

For the $\mathcal{O}(\beta_0^3\alpha_s^3)$ term we obtain

$$\delta^{(3)}_{\beta_0^3}E_1 = E_1^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[32L_1^3+40L_1^2+\left(\frac{16\pi^2}{3}+64\zeta(3)\right)L_1$$

$$-8+4\pi^2+\frac{2\pi^4}{45}+64\zeta(3)-8\pi^2\zeta(3)+96\zeta(5)\Bigg],$$

$$\begin{aligned}
\delta^{(3)}_{\beta_0^3}E_2 &= E_2^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[32L_2^3+88L_2^2+\left(32+\frac{16\pi^2}{3}+128\zeta(3)\right)L_2 \\
&\quad -102+\frac{52\pi^2}{3}+\frac{4\pi^4}{45}+112\zeta(3)-32\pi^2\zeta(3)+384\zeta(5)\Bigg], \\
\delta^{(3)}_{\beta_0^3}E_3 &= E_3^C\left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[32L_3^3+120L_3^2+\left(\frac{136}{3}+\frac{16\pi^2}{3}+192\zeta(3)\right)L_3 \\
&\quad -\frac{9514}{27}+\frac{427\pi^2}{9}+\frac{2\pi^4}{15}+140\zeta(3)-72\pi^2\zeta(3)+864\zeta(5)\Bigg], \qquad (4)
\end{aligned}$$

where $L_n=\ln(n\mu/(C_F\alpha_s(\mu)m_q))$ and $\zeta(5)=1.036927\ldots$. Note that the $n=1$ result has already been known [26,27,6]. The perturbative expansion for the wave function can be written as follows

$$|\psi_n(0)|^2 = |\psi_n^C(0)|^2\left(1+\delta^{(1)}\psi_n+\delta^{(2)}\psi_n+\delta^{(3)}\psi_n+\ldots\right), \qquad (5)$$

where

$$|\psi_n^C(0)|^2 = \frac{C_F^3\alpha_s^3m_q^3}{8\pi n^3}, \qquad (6)$$

is the leading order Coulomb value. Our result for the $\mathcal{O}(\beta_0^3\alpha_s^3)$ term reads

$$\begin{aligned}
\delta^{(3)}_{\beta_0^3}\psi_1 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[80L_1^3+\left(52-\frac{80\pi^2}{3}\right)L_1^2+\left(-40-6\pi^2+\frac{10\pi^4}{9}+200\zeta(3)\right)L_1 \\
&\quad -20+\frac{22\pi^2}{3}-\frac{7\pi^4}{5}+\frac{4\pi^6}{105}+112\zeta(3)-12\pi^2\zeta(3)-16\zeta(3)^2-40\zeta(5)\Bigg], \\
\delta^{(3)}_{\beta_0^3}\psi_2 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[80L_2^3+\left(332-\frac{160\pi^2}{3}\right)L_2^2+\left(308-\frac{266\pi^2}{3}+\frac{40\pi^4}{9}+400\zeta(3)\right)L_2 \\
&\quad -361+\frac{73\pi^2}{3}-\frac{26\pi^4}{45}+\frac{32\pi^6}{105}+496\zeta(3)-48\pi^2\zeta(3)-128\zeta(3)^2-160\zeta(5)\Bigg], \\
\delta^{(3)}_{\beta_0^3}\psi_3 &= \left(\frac{\beta_0\alpha_s}{\pi}\right)^3\Bigg[80L_3^3+\left(612-80\pi^2\right)L_3^2+\left(\frac{2893}{3}-228\pi^2+10\pi^4+600\zeta(3)\right)L_3 \\
&\quad -\frac{100679}{54}+\frac{183\pi^2}{2}+\frac{52\pi^4}{15}+\frac{36\pi^6}{35}+1374\zeta(3)-108\pi^2\zeta(3)-432\zeta(3)^2 \\
&\quad -360\zeta(5)\Bigg]. \qquad (7)
\end{aligned}$$

3 Exited states spectrum to $\mathcal{O}(m_q\alpha_s^5)$

The heavy quarkonium spectrum up to $\mathcal{O}(m_q\alpha_s^4)$ has been derived in Refs. [28,7,8]. For convenience of the reader the expressions for $\delta E_n^{(1)}$ and $\delta E_n^{(2)}$ are listed in Appendix B.

At $\mathcal{O}(m_q\alpha_s^5)$ it is convenient to split $\delta E_n^{(3)}$ into two parts: one corresponding to vanishing beta-function and one proportional to the coefficients of beta-function:

$$\delta E_n^{(3)} = \delta E_n^{(3)}\Big|_{\beta(\alpha_s)=0} + \delta E_n^{(3)}\Big|_{\beta(\alpha_s)}. \tag{8}$$

The contribution $\delta E_n^{(3)}\Big|_{\beta(\alpha_s)=0}$ has been evaluated in Ref. [21]. For completeness we include the corresponding expressions in Appendix B. In Ref. [6] the quantity $\delta E_n^{(3)}\Big|_{\beta(\alpha_s)}$ has been computed for $n = 1$. Below we extend it to the excited states. Following Ref. [6] we divide $\delta E_n^{(3)}\Big|_{\beta(\alpha_s)}$ into four pieces

$$\delta E_n^{(3)}\Big|_{\beta(\alpha_s)} = \delta E_n^{(3)}\Big|_{\rm C.r.} + \delta E_n^{(3)}\Big|_{\rm B.r.} + \delta E_n^{(3)}\Big|_{\rm C.i.} + \delta E_n^{(3)}\Big|_{\rm B.i.}. \tag{9}$$

The first two terms of the above equation are related to the running of the lower-order potentials. The contribution $\delta E_n^{(3)}\Big|_{\rm C.r.}$ is due to the three-loop running of the static potential, Eq. (1). It reads

$$\begin{aligned}
\delta E_n^{(3)}\Big|_{\rm C.r.} &= E_n^C \left(\frac{\alpha_s(\mu)}{\pi}\right)^3 \Bigg\{ \left(6a_1\beta_0^2 + 20\beta_0\beta_1\right) L_n^2 + \Bigg(12P_{n+1}a_1\beta_0^2 + \frac{3}{4}a_2\beta_0 + 2a_1\beta_1 \\
&\quad + 40P_{n+1}\beta_0\beta_1 + 4\beta_2\Bigg) L_n + \left(-\frac{12}{n^2} + \frac{5\pi^2}{2} - \frac{12}{n}P_n + 6P_{n+1}^2 - 6\Psi_2(n+1)\right) \\
&\quad \times a_1\beta_0^2 + \frac{3}{4}P_{n+1}a_2\beta_0 + 2P_{n+1}a_1\beta_1 + \Bigg(-\frac{40}{n^2} + \frac{25\pi^2}{3} - \frac{40}{n}P_n + 20P_{n+1}^2 \\
&\quad - 20\Psi_2(n+1)\Bigg)\beta_0\beta_1 + 4P_{n+1}\beta_2 \Bigg\} + \delta^{(3)}_{\beta_0^3} E_n\Big|_{\rm C.r.},
\end{aligned} \tag{10}$$

where $P_n = \Psi_1(n)+\gamma_E$, $\Psi_n(z) = {\rm d}^n \ln(\Gamma(z))/{\rm d}z^n$ and $\Gamma(z)$ is the Euler's gamma-function. The term $\delta^{(3)}_{\beta_0^3} E_n\Big|_{\rm C.r.}$ in Eq. (10) is included in Eq. (4).

The contribution $\delta E_n^{(3)}\Big|_{\rm B.r.}$ is due to the one-loop running of the power suppressed terms in the NNLO[1] effective Hamiltonian (see, e.g., Ref. [21]), which we denote as the "Breit potential". For this contribution we obtain

$$\begin{aligned}
\delta E_n^{(3)}\Big|_{\rm B.r.} &= E_n^C \frac{\alpha_s^3(\mu)}{\pi}\beta_0 \Bigg\{ \left[\frac{4}{n}C_FC_A + \left(2 - \frac{1}{n} - \frac{4}{3}S(S+1)\right)\frac{C_F^2}{n}\right] L_n \\
&\quad + (4 - 4P_{n+1})\frac{C_FC_A}{n} + \Bigg[\left(2 - \left(2+\frac{1}{n}\right)P_{n+1}\right) \\
&\quad + \left(-\frac{2}{3n} + \frac{2}{3} + \frac{4}{3}P_{n+1}\right) S(S+1)\Bigg]\frac{C_F^2}{n} \Bigg\},
\end{aligned} \tag{11}$$

where S is the spin quantum number.

[1]LO, NLO, ... stand for the leading order, next-to-leading order, *etc.*

The remaining two contributions of Eq. (9) are related to the iteration of lower-order potentials. The contribution $\delta E_n^{(3)}\Big|_{\rm C.r.}$ corresponds to the iteration of the one- and two-loop running of the static potential and is of the following form

$$
\begin{aligned}
\delta E_n^{(3)}\Big|_{\rm C.i.} &= E_n^C \left(\frac{\alpha_s(\mu)}{\pi}\right)^3 \Bigg\{ \left(6a_1\beta_0^2 + 8\beta_0\beta_1\right) L_n^2 + \Bigg[\frac{a_1^2\beta_0}{2} + \frac{a_2\beta_0}{4} \\
&\quad + \left(-14 + \frac{12}{n} + 12P_n\right) a_1\beta_0^2 + a_1\beta_1 + \left(-16 + \frac{16}{n} + 16P_n\right)\beta_0\beta_1\Bigg] L_n \\
&\quad + \left(-\frac{5}{8} + \frac{1}{2n} + \frac{P_n}{2}\right) a_1^2\beta_0 + \left(-\frac{1}{4} + \frac{1}{4n} + \frac{P_n}{4}\right) a_2\beta_0 + \Bigg[2 + \frac{12}{n^2} - \frac{14}{n} + \frac{5\pi^2}{6} \\
&\quad + \left(-14 + \frac{16}{n}\right) P_n + 6P_n^2 - 10\Psi_2(n) - 4n\Psi_3(n)\Bigg] a_1\beta_0^2 + \left(-1 + \frac{1}{n} + P_n\right) \\
&\quad \times a_1\beta_1 + \Bigg[\frac{24}{n^2} - \frac{16}{n} + \left(-16 + \frac{32}{n}\right) P_n + 8P_n^2 - 16\Psi_2(n) - 8n\Psi_3(n)\Bigg]\beta_0\beta_1\Bigg\} \\
&\quad + \delta_{\beta_0^3}^{(3)} E_n\Big|_{\rm C.i.}\,,
\end{aligned}
\tag{12}
$$

where $\delta_{\beta_0^3}^{(3)} E_n\Big|_{\rm C.i.}$ contributes to Eq. (4).

The last contribution $\delta E_n^{(3)}\Big|_{\rm B.i.}$ incorporates the iteration of the Breit potential and the one-loop running of the static potential. It reads

$$
\begin{aligned}
\delta E_n^{(3)}\Big|_{\rm B.i.} &= E_n^C \frac{\alpha_s^3(\mu)}{\pi}\beta_0 \Bigg\{\Bigg[\frac{4}{n}C_F C_A + \left(-\frac{9}{2n} + 14 - 4S(S+1)\right)\frac{C_F^2}{n}\Bigg] L_n \\
&\quad + \left(\frac{4}{n^2} - \frac{2}{n} + \frac{4}{n}P_{n+1} - 4\Psi_2(n)\right) C_F C_A + \Bigg[\frac{19}{2n^2} + \frac{2}{n} + \left(-\frac{9}{2n^2} + \frac{2}{n}\right) P_{n+1} \\
&\quad -8\Psi_2(n) + \left(-\frac{8}{3n^2} + \frac{4}{3n} - \frac{4}{3n}P_{n+1} + \frac{8}{3}\Psi_2(n)\right) S(S+1)\Bigg] C_F^2\Bigg\}\,.
\end{aligned}
\tag{13}
$$

After summing up the four contributions according to Eq. (9) we obtain our final result for the $\mathcal{O}(\alpha_s^3)$ corrections to the energy levels involving coefficients of the beta function. For $n = 1,\ 2$, and 3 they read

$$
\begin{aligned}
\delta E_1^{(3)}\Big|_{\beta(\alpha_s)} &= E_1^C \left(\frac{\alpha_s(\mu)}{\pi}\right)^3 \Bigg\{ 32\beta_0^3 L_1^3 + \left(12a_1\beta_0^2 + 40\beta_0^3 + 28\beta_0\beta_1\right) L_1^2 \\
&+ \Bigg[\frac{a_1^2\beta_0}{2} + a_2\beta_0 + 10a_1\beta_0^2 + \left(\frac{16\pi^2}{3} + 64\zeta(3)\right)\beta_0^3 + 3a_1\beta_1 + 40\beta_0\beta_1 + 4\beta_2 \\
&+ 8\pi^2\beta_0 C_F C_A + \left(\frac{21}{2} - \frac{16}{3}S(S+1)\right)\pi^2\beta_0 C_F^2\Bigg] L_1 - \frac{a_1^2\beta_0}{8} + \frac{3}{4}a_2\beta_0 + \left(\frac{2\pi^2}{3} + 8\zeta(3)\right) \\
&\times a_1\beta_0^2 + \Bigg[-8 + \frac{2\pi^4}{45} + (4 - 8\zeta(3))\,\pi^2 + 64\zeta(3) + 96\zeta(5)\Bigg]\beta_0^3 + 2a_1\beta_1 \\
&+ \left(8 + \frac{7\pi^2}{3} + 16\zeta(3)\right)\beta_0\beta_1 + 4\beta_2 + \left(6 - \frac{2\pi^2}{3}\right)\pi^2\beta_0 C_F C_A + \Bigg[8 - \frac{4\pi^2}{3}
\end{aligned}
$$

$$+\left(-\frac{4}{3}+\frac{4\pi^2}{9}\right)S(S+1)\bigg]\pi^2\beta_0C_F^2\bigg\}\,,$$

$$\delta E_2^{(3)}\Big|_{\beta(\alpha_s)} = E_2^C\left(\frac{\alpha_s(\mu)}{\pi}\right)^3\bigg\{32\beta_0^3L_2^3+\left(12a_1\beta_0^2+88\beta_0^3+28\beta_0\beta_1\right)L_2^2$$
$$+\bigg[\frac{a_1^2\beta_0}{2}+a_2\beta_0+22a_1\beta_0^2+\left(32+\frac{16\pi^2}{3}+128\zeta(3)\right)\beta_0^3+3a_1\beta_1+68\beta_0\beta_1+4\beta_2$$
$$+4\pi^2\beta_0C_FC_A+\left(\frac{53}{8}-\frac{8}{3}S(S+1)\right)\pi^2\beta_0C_F^2\bigg]L_2+\frac{a_1^2\beta_0}{8}+\frac{5}{4}a_2\beta_0+\bigg(4+\frac{2\pi^2}{3}$$
$$+16\zeta(3)\bigg)a_1\beta_0^2+\left[-102+\frac{4\pi^4}{45}+\left(\frac{52}{3}-32\zeta(3)\right)\pi^2+112\zeta(3)+384\zeta(5)\right]\beta_0^3$$
$$+\frac{7}{2}a_1\beta_1+\left(30+\frac{7\pi^2}{3}+32\zeta(3)\right)\beta_0\beta_1+6\beta_2+\left(6-\frac{2\pi^2}{3}\right)\pi^2\beta_0C_FC_A+\bigg[\frac{165}{16}-\frac{4\pi^2}{3}$$
$$+\left(-\frac{5}{2}+\frac{4\pi^2}{9}\right)S(S+1)\bigg]\pi^2\beta_0C_F^2\bigg\}\,,$$

$$\delta E_3^{(3)}\Big|_{\beta(\alpha_s)} = E_3^C\left(\frac{\alpha_s(\mu)}{\pi}\right)^3\bigg\{32\beta_0^3L_3^3+\left(12a_1\beta_0^2+120\beta_0^3+28\beta_0\beta_1\right)L_3^2$$
$$+\bigg[\frac{a_1^2\beta_0}{2}+a_2\beta_0+30a_1\beta_0^2+\left(\frac{136}{3}+\frac{16\pi^2}{3}+192\zeta(3)\right)\beta_0^3+3a_1\beta_1+\frac{260}{3}\beta_0\beta_1+4\beta_2$$
$$+\frac{8\pi^2}{3}\beta_0C_FC_A+\left(\frac{85}{18}-\frac{16}{9}S(S+1)\right)\pi^2\beta_0C_F^2\bigg]L_3+\frac{7}{24}a_1^2\beta_0+\frac{19}{12}a_2\beta_0+\bigg(\frac{17}{3}+\frac{2\pi^2}{3}$$
$$+24\zeta(3)\bigg)a_1\beta_0^2+\left[-\frac{9514}{27}+\frac{2\pi^4}{15}+\left(\frac{427}{9}-72\zeta(3)\right)\pi^2+140\zeta(3)+864\zeta(5)\right]\beta_0^3$$
$$+\frac{9}{2}a_1\beta_1+\left(\frac{130}{3}+\frac{7\pi^2}{3}+48\zeta(3)\right)\beta_0\beta_1+\frac{22}{3}\beta_2+\left(\frac{55}{9}-\frac{2\pi^2}{3}\right)\pi^2\beta_0C_FC_A$$
$$+\left[\frac{1217}{108}-\frac{4\pi^2}{3}+\left(-\frac{82}{27}+\frac{4\pi^2}{9}\right)S(S+1)\right]\pi^2\beta_0C_F^2\bigg\}\,. \qquad (14)$$

The equation with $n=1$ agrees with the result of Ref. [6]. The Eqs. (14), (25), (26) and (27) provide the complete result for the energy levels up to $\mathcal{O}(m_q\alpha_s^5)$. We should note that, although we only present analytical results for the first three principle quantum numbers, there is no principle problem to obtain expressions for higher excited states, too. However, from the phenomenological point of view they are far less important, and thus we refrain from listing them explicitly.

It is instructive to evaluate the energy levels in numerical form:

$$\frac{\delta E_1^{(3)}}{E_1^C} = \alpha_s^3\left[\begin{pmatrix} 70.590|_{n_l=4} \\ 56.732|_{n_l=5}\end{pmatrix}+15.297\ln\alpha_s+0.001\,a_3+\begin{pmatrix} 34.229|_{n_l=4} \\ 26.654|_{n_l=5}\end{pmatrix}\bigg|_{\beta_0^3}\right]\,,$$
$$\frac{\delta E_2^{(3)}}{E_2^C} = \alpha_s^3\left[\begin{pmatrix} 84.634|_{n_l=4} \\ 62.164|_{n_l=5}\end{pmatrix}+8.647\ln\alpha_s+0.001\,a_3+\begin{pmatrix} 67.337|_{n_l=4} \\ 52.434|_{n_l=5}\end{pmatrix}\bigg|_{\beta_0^3}\right]\,,$$

$$\frac{\delta E_3^{(3)}}{E_3^C} = \alpha_s^3 \left[\left(\begin{array}{c} 101.69|_{n_l=4} \\ 72.368|_{n_l=5} \end{array} \right) + 6.305 \ln \alpha_s + 0.001\, a_3 + \left(\begin{array}{c} 98.824|_{n_l=4} \\ 76.953|_{n_l=5} \end{array} \right) \Bigg|_{\beta_0^3} \right] , \quad (15)$$

where $\alpha_s = \alpha_s(\mu_s/n)$ and $\mu = \mu_s/n$ with $\mu_s = C_F \alpha_s(\mu_s) m_q$ and we put $S = 1$ which corresponds to the spin-triplet state. The recent analysis of the spin-dependent contribution to the spectrum, which is responsible for the hyperfine splitting, can be found in Refs. [29,30]. In Eq. (15) we have separated the contributions arising from a_3 and β_0^3. Using the Padé estimates [23] we obtain $0.001\, a_3|_{n_l=4} \approx 6$ and $0.001\, a_3|_{n_l=5} \approx 4$. Thus, the result for the energy levels depends only marginally on the precise value of a_3 provided the Padé estimates give the correct order of magnitude. Furthermore, one can see that the β_0^3 term contributes between 25% ($n = 1$) and 50% ($n = 3$) of the nonlogarithmic term.

4 Heavy quarkonium phenomenology

In this section we discuss some phenomenological applications of the results derived in the previous parts of the paper. As input values for the numerical analyses we adopt $\alpha_s(M_Z) = 0.118$, and $m_b = 5.3$ GeV and $m_t = 175$ GeV for the quark pole masses. Furthermore, we use the soft scale $\mu_s \approx 2.10$ GeV for the bottom and $\mu_s \approx 32.6$ GeV for the top quark case.

Excited states of bottomonium. The mass of the $\Upsilon(nS)$ meson can be decomposed into perturbative and nonperturbative contributions

$$M_{\Upsilon(nS)} = 2m_b + E_n^{\text{p.t.}} + \delta^{\text{n.p.}} E_n \,. \quad (16)$$

The perturbative contribution $E_n^{\text{p.t.}}$ up to $\mathcal{O}(m_q \alpha_s^5)$ is given in the previous sections. The phenomenological application of the result to the $\Upsilon(1S)$ meson mass has been discussed in Ref. [6]. For the exited states let us consider the ratio

$$\rho_n = \frac{E_n - E_1}{2m_b + E_1} \,. \quad (17)$$

It depends on the quark mass only through the normalization scale of α_s and does not suffer from renormalon contributions. Including successively higher orders one gets for $\mu = \mu_s$

$$\begin{aligned} 10^2 \times \rho_2^{\text{p.t.}} &= 1.49\,(1 + 0.79_{\text{NLO}} + 1.18_{\text{NNLO}} + 1.21_{\text{N}^3\text{LO}} + \ldots) \,, \\ 10^2 \times \rho_3^{\text{p.t.}} &= 1.77\,(1 + 0.92_{\text{NLO}} + 1.37_{\text{NNLO}} + 1.55_{\text{N}^3\text{LO}} + \ldots) \,, \end{aligned} \quad (18)$$

where $\alpha_s^{(4)}(\mu_s)$ is extracted from its value at M_Z using four-loop beta-function accompanied with three-loop matching[2]. Though the convergence of the series is not good,

[2] We use the package RunDec [31] to perform the running and matching of α_s.

	$\Upsilon(2S)$	$\Upsilon(3S)$
$10^2 \times \rho_n^{\rm p.t.}$	$6.2^{+1.7}_{-1.2}$	$8.6^{+2.4}_{-1.8}$
$10^2 \times \rho_n^{\rm exp}$	5.95	9.46

Table 1: Perturbative versus experimental results for the parameter ρ_n as defined in Eq. (17). The theoretical uncertainty corresponds to $\alpha_s(M_Z) = 0.118 \pm 0.003$. The experimental values are extracted from Ref. [34]. For a_3 we used the Padé estimate [23] $a_3|_{n_l=4} = 6272$.

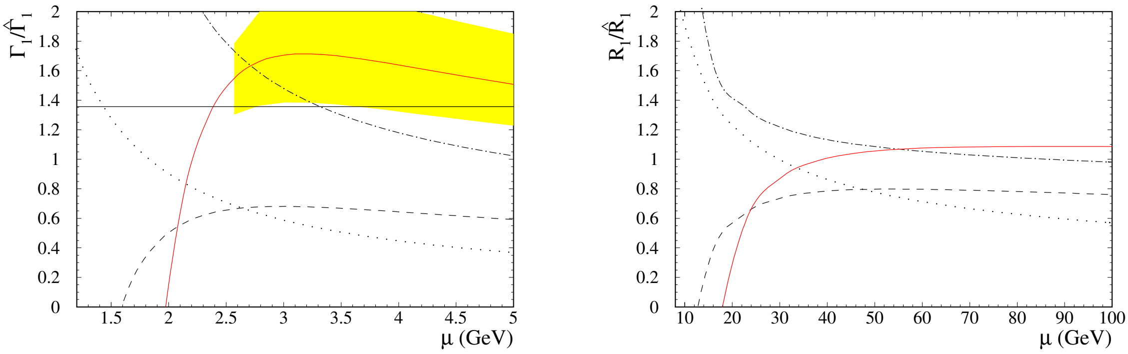
the N^{3}LO perturbative result is in impressive agreement with the experimental values $\rho_n^{\rm exp} = (M_{\Upsilon(nS)} - M_{\Upsilon(1S)})/M_{\Upsilon(1S)}$ for $n = 2$ and 3 as can be seen in Tab. 1. We would like to emphasize the role of the perturbative corrections necessary to bring theory and experiment into agreement which we will use in the following to estimate the order of magnitude of the nonperturbative effects. In fact the absence of a sufficiently accurate estimate of the nonperturbative part $\delta^{\rm n.p.}E_n$ is one of the main problems in the theory of heavy quarkonium. In the limit $\alpha_s^2 m_q \gg \Lambda_{QCD}$ it can be investigated by the method of vacuum condensate expansion [4,5]. However, for bottomonium it can only be used for $n = 1$. For higher states the leading term due to the gluonic condensate grows as n^6. It becomes unacceptably large already for $n = 2$ where the whole series blows up [32]. Even for $n = 1$ such an estimate suffers from large uncertainties due to the poorly known value of the gluonic condensate and due to a strong scale dependence. A rough numerical estimate is $\delta^{\rm n.p.}E_1 \approx 60$ MeV [6]. Since our perturbative result agrees very well with the experimental result we can conclude that $\delta^{\rm n.p.}E_2$ should be of the same size as $\delta^{\rm n.p.}E_1$. In general for bottomonium the nonperturbative corrections appear to be rather moderate and the theoretical estimates are dominated by perturbative contributions. Similar conclusion has been made in Ref. [33] in a somewhat different framework.

$\Upsilon(1S)$ **leptonic width.** In the nonrelativistic effective theory the leading order approximation for the leptonic width $\Gamma^{\rm LO}(\Upsilon(1S) \to l^+l^-) \equiv \Gamma_1$ reads $\Gamma_1^{\rm LO} = 4\pi N_c Q_b^2 \alpha^2 |\psi_1^C(0)|^2/(3m_b^2)$, with $N_c = 3$ and $Q_b = -1/3$. Combining the known perturbative results up to $\mathcal{O}(\alpha_s^3 \ln\alpha_s)$ (see Ref. [12]) with the $\mathcal{O}(\beta_0^3\alpha_s^3)$ contribution obtained in Section 2 we obtain the following series

$$\begin{aligned} \Gamma_1 \;\approx\;& \Gamma_1^{\rm LO}\Big(1 - 1.70\,\alpha_s(m_b) - 7.98\,\alpha_s^2(m_b) + \ldots\Big) \\ &\times\Big(1 - 0.30\,\alpha_s - 5.19\,\alpha_s^2\ln\alpha_s + 17.2\,\alpha_s^2 \\ &-14.4\,\alpha_s^3\ln^2\alpha_s + 0.17\,\alpha_s^3\ln\alpha_s - 34.9\,\alpha_s^3|_{\beta_0^3} + \ldots\Big)\,, \end{aligned} \tag{19}$$

where $\alpha_s = \alpha_s(\mu_s)$. The contribution coming from the hard virtual momenta region [35,36] is separated and the corresponding strong coupling is normalized at $\mu = m_b$. Evaluating Eq. (19) and retaining only the logarithmic and β_0^3 terms at N^{3}LO we find

$$\Gamma_1 \;\approx\; \Gamma_1^{\rm LO}(1 - 0.445_{\rm NLO} + 1.75_{\rm NNLO} - 1.67_{\rm N^3LO'} + \ldots)\,, \tag{20}$$



(a) (b)

Figure 1: (a) Γ_1 normalized to $\hat{\Gamma}_1 \equiv \Gamma_1^{\rm LO}|_{\alpha_s\to\alpha_s(\mu_s)}$ as a function of μ at LO (dotted), NLO (dashed), NNLO (dotted-dashed) and N^{3}LO$'$ (full line). The horizontal line corresponds to the experimental value $\Gamma^{\rm exp}(\Upsilon(1S) \to e^+e^-) = 1.31$ keV [34]. For the N^{3}LO$'$ result, the band reflects the errors due to $\alpha_s(M_Z) = 0.118 \pm 0.003$. (b) The analog plot for R_1 with $\hat{R}_1 \equiv R_1^{\rm LO}|_{\alpha_s\to\alpha_s(\mu_s)}$.

where the prime indicates that the N^{3}LO corrections are not complete. Though the perturbative corrections are huge, the rapid growth of the perturbative coefficients stops at NNLO if we assume that the β_0^3 term sets the scale of the nonlogarithmic third-order contribution. In Fig. 1(a), the width is plotted as a function of μ including the LO, NLO, NNLO and N^{3}LO$'$ approximations along with the experimental value. For the numerical evaluation we extract $\alpha_s^{(4)}(m_b)$ from its value at M_Z using four-loop beta-function accompanied with three-loop matching. $\alpha_s^{(4)}(m_b)$ is used as starting point in order to evaluate $\alpha_s^{(4)}(\mu)$ at N^{k}LO with the help of the $(k+1)$-loop beta-function. As one can see in Fig. 1(a), the available $\mathcal{O}(\alpha_s^3)$ terms stabilize the series and significantly reduce the scale dependence. At the scale $\mu' \approx 2.7$ GeV, which is close to the physically motivated scale μ_s, the N^{3}LO$'$ corrections vanish and at the scale $\mu'' \approx 3.1$ GeV the result becomes independent of μ; *i.e.*, the N^{3}LO$'$ curve shows a local maximum. In the whole range of μ between 2 GeV and 5 GeV the result for the width agrees with the experimental value within the error bar due to the uncertainty of the strong coupling constant. This may signal that the missing perturbative corrections are rather moderate. Furthermore, this result constitutes a significant improvement as compared to the NLL approximation discussed in Ref. [37].

For a definite conclusion, however, one has to wait until the third-order corrections are completed. The potentially most important part to be computed is the ultrasoft contribution which includes $\alpha_s(\mu)$ normalized at relatively low ultrasoft scale $\mu_{us} \sim \alpha_s^2 m_q$. Currently only a partial result for this contribution exists [38].

Υ sum rules. The nonrelativistic Υ sum rules [2] operate with the high moments of the spectral density with $n \sim 1/\alpha_s^2$, which are saturated by the nonrelativistic nearthreshold region. The experimental input is given by the masses and leptonic width of the Υ resonances which are known with high accuracy. On the theoretical side the nonperturbative effects are well under control. This makes the Υ sum rules one of the most accurate sources for the bottom quark mass value. The complete perturbative analysis has been performed up to NNLO [24,7,16,39,27]. The extension to N^{3}LO is a challenging problem.

The theoretical value of the high moments is saturated by the contribution of a few lowest heavy quarkonium states and the corrections to the moments are dominated by the corrections to their masses and wave functions at the origin. To estimate the size of the N^{3}LO corrections we include the $\mathcal{O}(m_q\alpha_s^5)$ result for the energy levels and the partial $\mathcal{O}(\alpha_s^3)$ result for the wave function at the origin which includes all the logarithmic term [12] and the β_0^3 terms obtained in Section 3. We perform the analysis along the lines described in Ref. [7] using $\mu = \mu_s$. For $n \geq 20$ the corrections to the moments are dominated by the one to the ground state energy and we recover the result of Ref. [6] for the bottom quark mass. For lower moments, which provide better balance between theoretical end experimental uncertainties [7], the situation changes drastically as the corrections to the wave function at the origin begin to play an important role. For $n = 4$ the negative third-order contribution to the wave function completely cancels the effect of the third-order correction to the binding energy, and the correction to the pole mass m_b almost vanishes. The pole mass can be converted into the $\overline{\rm MS}$ mass $\bar{m}_b(\bar{m}_b)$ which is widely believed to have much better perturbative properties. If we correlate the series so that the $k^{\rm th}$-order correction to the sum rules goes along with the k-loop mass relation, which is natural for low moments, we obtain as an effect of the third-order corrections $\delta\bar{m}_b(\bar{m}_b)_{\rm N^3LO} \approx -100$ MeV. We take this variation as an estimate for the size of the N^{3}LO corrections within the Υ sum-rule approach. It is interesting to note that the N^{3}LO correction to $\bar{m}_b(\bar{m}_b)$ is *negative* at the soft normalization scale in contrast to the series obtained from the ground state energy analysis [6].

Top quark-antiquark threshold production. The nonperturbative effects in the case of the top quark are negligible. However, due to the relatively large top quark width, Γ_t, its effect has to be taken into account properly [3] since the Coulomb-like resonances below threshold are smeared out. Actually, the cross section only shows a small bump which is essentially the remnant of the ground state pole. The higher poles and continuum, however, affect the position of the resonance peak and move it to higher energy. The value of the normalized cross section $R = \sigma(e^+e^- \to t\bar{t})/\sigma(e^+e^- \to \mu^+\mu^-)$ at the resonance energy is dominated by the contribution from the *would-be* toponium ground state which in the leading approximation reads $R_1^{\rm LO} = 6\pi N_c Q_t^2 |\psi_1^C(0)|^2/\,(m_t^2\Gamma_t)$, where $Q_t = 2/3$. The analog to Eq. (19) reads

$$\begin{aligned} R_1 \;\approx\;& R_1^{\rm LO}\Big(1 - 1.70\,\alpha_s(m_t) - 7.89\,\alpha_s^2(m_t) + \ldots\Big) \\ &\times\Big(1 - 0.43\,\alpha_s - 5.19\,\alpha_s^2\ln\alpha_s + 16.1\,\alpha_s^2 \\ &-13.8\,\alpha_s^3\ln^2\alpha_s + 2.06\,\alpha_s^3\ln\alpha_s - 27.2\,\alpha_s^3|_{\beta_0^3} + \ldots\Big)\,, \end{aligned} \qquad (21)$$

with $\alpha_s = \alpha_s(\mu_s)$. Numerically we find

$$R_1 \approx R_1^{\rm LO}(1 - 0.243_{\rm NLO} + 0.435_{\rm NNLO} - 0.268_{\rm N^3LO'} + \ldots)\,. \tag{22}$$

The new third-order corrections proportional to β_0^3 amount to approximately -7% of the LO approximation at the soft scale which is the same order of magnitude as the $\mathcal{O}(\alpha_s^3)$ linear logarithmic term. The available N^{3}LO terms improve the stability of the result with respect to the scale variation as can be seen in Fig. 1(b). The absence of a rapid growth of the coefficients along with the alternating-sign character of the series and the weak scale dependence suggest that the missing perturbative corrections are moderate and most likely are in the few-percent range. It is interesting to note that the perturbative contributions of different orders, which are relatively large when taken separately, cancel in the sum to give only a few percent variation of the leading order result.

5 Summary

In this paper the important class of the third-order corrections to the heavy quarkonium parameters proportional to β_0^3 has been obtained. The complete result for the exited states spectrum to $\mathcal{O}(m_q\alpha_s^5)$ is derived. The perturbative results are in surprisingly good agreement with the $\Upsilon(2S)$ and $\Upsilon(3S)$ meson masses and the leptonic width of the $\Upsilon(1S)$ meson. Thus the nonperturbative effects in bottomonium seem to be rather moderate and the theoretical results are dominated by the perturbative contributions. A failure of early low-order perturbative analysis to describe the Υ system is due to large perturbative corrections to the Coulomb approximation. On the basis of our results the magnitude of the N^{3}LO corrections to the Υ sum rules and top quark-antiquark threshold production cross section is estimated. The available N^{3}LO corrections which include all logarithmic terms and the nonlogarithmic β_0^3 contribution stabilize the perturbative series for the production/annihilation rates that makes us more optimistic about possible accurate perturbative description of these quantities.

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A Static potential and beta-function

For convenience of the reader we list in this appendix the result for the coefficients of the static potential (see [41–43] and references therein)

$$
\begin{aligned}
a_1 &= \frac{31}{9}C_A - \frac{20}{9}T_F n_l\,, \\
a_2 &= \left[\frac{4343}{162} + 4\pi^2 - \frac{\pi^4}{4} + \frac{22}{3}\zeta(3)\right]C_A^2 - \left[\frac{1798}{81} + \frac{56}{3}\zeta(3)\right]C_A T_F n_l \\
&\quad - \left[\frac{55}{3} - 16\zeta(3)\right]C_F T_F n_l + \left(\frac{20}{9}T_F n_l\right)^2\,,
\end{aligned}
\tag{23}
$$

and the beta-function

$$
\begin{aligned}
\beta_0 &= \frac{1}{4}\left(\frac{11}{3}C_A - \frac{4}{3}T_F n_l\right)\,, \\
\beta_1 &= \frac{1}{16}\left(\frac{34}{3}C_A^2 - \frac{20}{3}C_A T_F n_l - 4C_F T_F n_l\right)\,, \\
\beta_2 &= \frac{1}{64}\left(\frac{2857}{54}C_A^3 - \frac{1415}{27}C_A^2 T_F n_l - \frac{205}{9}C_A C_F T_F n_l + 2C_F^2 T_F n_l + \frac{158}{27}C_A T_F^2 n_l^2\right. \\
&\quad \left. + \frac{44}{9}C_F T_F^2 n_l^2\right)\,,
\end{aligned}
\tag{24}
$$

where $T_F = 1/2$ and n_l is the number of the light quark flavours.

B Results for $\delta E_n^{(i)}$

In this appendix we collect the known results for the perturbative corrections to the heavy quarkonium spectrum. The first and the second order corrections read [28,7,8]

$$
\delta E_n^{(1)} = E_n^C \frac{\alpha_s}{\pi}\left[4\beta_0\left(L_n + P_{n+1}\right) + \frac{a_1}{2}\right]\,,
\tag{25}
$$

$$
\begin{aligned}
\delta E_n^{(2)} &= E_n^C \left(\frac{\alpha_s}{\pi}\right)^2 \left[12\beta_0^2 L_n^2 + \left(3a_1\beta_0 + 4\beta_1 + \left(-8 + 24P_{n+1}\right)\beta_0^2\right)L_n + \frac{a_1^2}{16} + \frac{a_2}{8}\right. \\
&\quad + \left(-1 + 3P_{n+1}\right)a_1\beta_0 + \left(\frac{8}{n^2} + \frac{10\pi^2}{3} - \left(8 + \frac{8}{n}\right)P_{n+1} + 12P_{n+1}^2\right. \\
&\quad \left. - 16\Psi_2(n) - 4n\Psi_3(n)\right)\beta_0^2 + 4P_{n+1}\beta_1 \\
&\quad \left. + \frac{\pi^2}{n}C_A C_F + \left(\frac{2}{n} - \frac{11}{16n^2} - \frac{2}{3n}S(S+1)\right)\pi^2 C_F^2\right]\,.
\end{aligned}
\tag{26}
$$

The result for $\delta E_n^{(3)}\Big|_{\beta(\alpha_s)=0}$ reads [21]

$$
\delta E_n^{(3)}\Big|_{\beta(\alpha_s)=0} =
$$

$$
\begin{aligned}
&-E_n^C \frac{\alpha_s^3}{\pi}\left\{-\frac{a_1 a_2 + a_3}{32\pi^2} + \left[-\frac{C_A C_F}{2} + \left(-\frac{7}{4} + \frac{9}{16n} + \frac{S(S+1)}{2}\right) C_F^2\right] \frac{a_1}{n}\right. \\
&+ \left[\frac{5}{36} + \frac{1}{6}\left(\ln 2 - \gamma_E - \ln n - \Psi_1(n+1) + L_{\alpha_s}\right)\right] C_A^3 \\
&+ \left[-\frac{97}{36} + \frac{4}{3}\left(\ln 2 + \gamma_E - \ln n + \Psi_1(n+1) + L_{\alpha_s}\right)\right] \frac{C_A^2 C_F}{n} \\
&+ \left[\left(-\frac{139}{36} + 4\ln 2 + \frac{7}{6}(\gamma_E - \ln n + \Psi_1(n+1)) + \frac{41}{6} L_{\alpha_s}\right)\right. \\
&+ \left(\frac{47}{24} + \frac{2}{3}\left(-\ln 2 + \gamma_E + \ln n + \Psi_1(n+1) - L_{\alpha_s}\right)\right) \frac{1}{n} \\
&+ \left.\left(\frac{107}{108} - \frac{7}{12n} + \frac{7}{6}(\gamma_E - \ln n + \Psi_1(n+1) - L_{\alpha_s})\right) S(S+1)\right] \frac{C_A C_F^2}{n} \\
&+ \left[\frac{79}{18} - \frac{7}{6n} + \frac{8}{3}\ln 2 + \frac{7}{3}(\gamma_E - \ln n + \Psi_1(n+1)) + 3L_{\alpha_s} - \frac{S(S+1)}{3}\right] \frac{C_F^3}{n} \\
&+ \left[-\frac{32}{15} + 2\ln 2 + (1 - \ln 2) S(S+1)\right] \frac{C_F^2 T_F}{n} \\
&\left. + \frac{49 C_A C_F T_F n_l}{36n} + \left[\frac{8}{9} - \frac{5}{18n} - \frac{10}{27} S(S+1)\right] \frac{C_F^2 T_F n_l}{n} + \frac{2}{3} C_F^3 L_n^E\right\}, \qquad (27)
\end{aligned}
$$

where $L_{\alpha_s} = -\ln(C_F \alpha_s)$ and L_n^E stands for the QCD Bethe logarithms with the numerical values [38]

$$
L_1^E = -81.5379\,, \qquad L_2^E = -37.6710\,, \qquad L_3^E = -22.4818\,. \qquad (28)
$$

The terms proportional to L_{α_s} have been computed for the first time in Ref. [44].

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