# Calculations of binding energies and masses of heavy quarkonia using renormalon cancellation

Carlos Contreras,* Gorazd Cvetič,† and Patricio Gaete‡
*Department of Physics, Universidad Técnica Federico Santa María, Valparaíso, Chile*
(Received 14 November 2003; published 18 August 2004)

We use various methods of Borel integration to calculate the binding ground energies and masses of $b\bar{b}$ and $t\bar{t}$ quarkonia. The methods take into account the leading infrared renormalon structure of the (hard+)soft part of the binding energies $E(s)$, and of the corresponding quark pole masses $m_q$, where the contributions of these singularities in $M(s)=2m_q+E(s)$ cancel. Beforehand, we carry out the separation of the binding energy into its (hard+)soft and ultrasoft parts. The resummation formalisms are applied to expansions of $m_q$ and $E(s)$ in terms of quantities which do not involve renormalon ambiguity, such as $\overline{\rm MS}$ mass $\bar{m}_q$ and $\alpha_s(\mu)$. The renormalization scales $\mu$ are different in calculations of $m_q$, $E(s)$ and $E(us)$. The mass $\bar{m}_b$ is extracted, and the binding energies $E_{t\bar{t}}$ and the peak (resonance) energies $E_{\rm res.}$ for $t\bar{t}$ production are obtained.

DOI: 10.1103/PhysRevD.70.034008 PACS number(s): 12.38.Bx, 12.38.Aw, 12.38.Cy

## I. INTRODUCTION

There has been a significant activity in calculation of binding energies and masses of heavy quarkonia $q\bar{q}$ in recent years. The calculations, based on perturbative expansions, are primarily due to the knowledge of up to N$^2$LO term ($\sim\alpha_s^3$) of the static quark-antiquark potential $V(r)$ [1,2] and partial knowledge of the N$^3$LO term there; the knowledge of the $1/m_q$ and $1/m_q^2$ correction terms ([3] and references therein) and the ultrasoft gluon contributions to a corresponding effective theory N$^3$LO Hamiltonian [3–5]; and the knowledge of the pole mass $m_q$ up to order $\sim\alpha_s^3$ [7,8]. Another impetus in these calculations was given by the observation of the fact that the contributions of the leading infrared (IR) renormalon singularities (at $b=1/2$) of the pole mass $m_q$ and of the static potential $V(r)$ cancel in the sum $2m_q+V(r)$ [9–11] (analogous cancellations were discovered and used in the physics of mesons with one heavy quark [12]). Consequently, this cancellation effect must be present also in the total quarkonium mass $M=2m_q+E_{q\bar{q}}$ [13,14], or more precisely, in $M(s)=2m_q+E(s)$ where $E(s)$ is the hard + soft part of the binding energy, i.e., the part which includes the contributions of relative quark-antiquark momenta $|k^0|,|\mathbf{k}|\gtrsim m_q\alpha_s$, i.e., soft/potential scales (predominant) and higher hard scales (smaller contributions). In addition, the binding energy has contribution $E_{q\bar{q}}(us)$ from the ultrasoft momenta regime $|k^0|,|\mathbf{k}|\sim m_q\alpha_s^2$. The ultrasoft contribution is not related to the $b=1/2$ renormalon singularity, since this singularity has to do with the behavior of the theory in the region which includes the hard ($\sim m_q$) and soft/potential ($\sim m_q\alpha_s$) scales.

In this work, we numerically calculate the binding ground energies $E_{q\bar{q}}$ (separately the *s* and the *us* parts) and the mass $(2m_q+E_{q\bar{q}})$ of the heavy $q\bar{q}$ system, by taking into account the leading IR renormalon structure of $m_q$ and $E_{q\bar{q}}(s)$, in the spirit of the works of Refs. [13,14]. We combine some features of these two references: (a) the mass that we use in the perturbation expansions is a renormalon-free mass [11,13,15–17] which we choose to be the $\overline{\rm MS}$ mass $\bar{m}_q \equiv \bar{m}_q(\mu=\bar{m}_q)$; (b) Borel integrations [14] are used to perform resummations. However, before resummations we perform separation of the soft/potential (*s*) and ultrasoft (*us*) part of the binding energies, and apply the renormalon-based Borel resummation only to the *s* part. The renormalization scales used in the Borel resummations are $\mu_h\sim m_q$ (hard scale) for $2m_q$, and $m_q\alpha_s\lesssim\mu_s<m_q$ for $E_{q\bar{q}}(s)$. The term corresponding to $E_{q\bar{q}}(us)$ is evaluated at $\mu_{us}\sim m_q\alpha_s^2$ whenever perturbatively possible. Further, the Borel resummations are performed in three different ways: (a) using a slightly extended version of the full bilocal expansion of the type introduced and used in Refs. [14,18]; (b) using a new "$\sigma$-regularized" full bilocal expansion introduced in the present work; (c) using the form of the Borel transform where the leading IR renormalon structure is a common factor of the transform [19,20] (we call it *R*-method). The Borel integrations for both $m_q$ and $E_{q\bar{q}}(s)$ are performed by the same prescription (generalized principal value PV [19–22]) so as to ensure the numerical cancellation of the renormalon contributions in the sum $2m_q+E_{q\bar{q}}(s)$. Furthermore, we demonstrate numerically that in the latter sum the residues at the renormalons are really consistent with the renormalon cancellation when a reasonable factorization scale parameter for the *s*-*us* separation is used, while they become inconsistent with the aforementioned cancellation when no such separation is used. The obtained numerical results allow us to extract the mass $\bar{m}_b$ from the known $\Upsilon(1S)$ mass of the $b\bar{b}$ system and to demonstrate that the *us* contribution is the major source of uncertainty. We present also the numerical results for the ground state binding energy for the scalar and vector toponium $t\bar{t}$.

In Sec. II we recapitulate the calculation of the pole mass $m_q$ in terms of $\bar{m}_q$ and $\alpha_s(\mu_h)$, and summarize the bilocal method of Refs. [14,18], with a slight extension in the renormalon-part of the Borel transform. In Sec. III we perform the separation of the binding ground energy into the

*Electronic address: carlos.contreras@usm.cl
†Electronic address: gorazd.cvetic@usm.cl
‡Electronic address: patricio.gaete@usm.cl

 

soft/potential ($s$) and the ultrasoft ($us$) part, and in Sec. IV we determine the $s$-$us$ factorization scale parameter so that the renormalon residue reproduced from $E_{q\bar{q}}(s)$ becomes consistent with the renormalon cancellation condition. In Sec. IV we further apply several methods of the Borel resummation to calculate $E_{b\bar{b}}(s)$ and $E_{t\bar{t}}(s)$: the aforementioned bilocal method, the new "$\sigma$-regularized" bilocal method, as well as the aforementioned $R$-method, and always using in the expansions $\overline{m}_q$ mass. We also estimate there the ultrasoft contributions to the binding energy. In Sec. V we compare the obtained results with some of the results recently published in the literature and draw conclusions about the main numerical features of our resummation procedure.

## II. POLE MASS

Here we redo the calculation of the pole mass $m_q$ in terms of the $\overline{\rm MS}$ renormalon-free mass $\overline{m}_q \equiv \overline{m}_q(\mu=\overline{m}_q)$ and of $\alpha_s(\mu,\overline{\rm MS})$, using elements of the approach of Ref. [13] and the bilocal expansion method of Refs. [14,18]. In the Borel integration, we choose the (generalized) principal value (PV) prescription [19–22]. The ratio $S=(m_q/\overline{m}_q-1)$ has perturbation expansion in $\overline{\rm MS}$ scheme which is at present known to order $\sim\alpha_s^3$ (Ref. [6] for $\sim\alpha_s$; [7] for $\sim\alpha_s^2$; [8] for $\sim\alpha_s^3$),

$$S\equiv\frac{m_q}{\overline{m}_q}-1=\frac{4}{3}a(\mu)[1+a(\mu)r_1(\mu)+a^2(\mu)r_2(\mu)+\mathcal{O}(a^3)], \tag{1a}$$

$$r_1(\mu)=\kappa_1+\beta_0 L_m(\mu), \tag{1b}$$

$$r_2(\mu)=\kappa_2+(2\kappa_1\beta_0+\beta_1)L_m(\mu)+\beta_0^2 L_m^2(\mu), \tag{1c}$$

$$(4/3)\kappa_1=6.248\beta_0-3.739, \tag{1d}$$

$$(4/3)\kappa_2=23.497\beta_0^2+6.248\beta_1+1.019\beta_0-29.94, \tag{1e}$$

where $L_m=\ln(\mu^2/\overline{m}_q^2)$, while $\beta_0=(11-2n_f/3)/4$ and $\beta_1=(102-38n_f/3)/16$ are the renormalization scheme independent coefficients with $n_f=n_\ell$ being the number of light active flavors (quarks with masses lighter than $m_q$). The natural renormalization scale here is $\mu=\mu_h\sim m_q$ (hard scale).

Therefore, the Borel transform $B_S(b)$ is known to order $\sim b^2$,

$$B_S(b;\mu)=\frac{4}{3}\left[1+\frac{r_1(\mu)}{1!\beta_0}b+\frac{r_2(\mu)}{2!\beta_0^2}b^2+\mathcal{O}(b^3)\right]. \tag{2}$$

It has renormalon singularities at $b=1/2,3/2,2,\ldots,-1,-2,\ldots$ [15,23,24]. The behavior of $B_S$ near the leading IR renormalon singularity $b=1/2$ is determined by the resulting renormalon ambiguity of $m_q$ which has to have the dimensions of energy and should be renormalization scale and scheme independent–the only such QCD scale being const$\times\Lambda_{\rm QCD}$ [25] (cf. also [18]). This scale is proportional to the Stevenson scale $\tilde{\Lambda}$ [26] (cf. also [27]). The latter can be obtained in terms of the strong coupling parameter $a(\mu;c_2,c_3,\ldots)=\alpha_s(\mu;c_2,c_3,\ldots)/\pi$, where $c_j=\beta_j/\beta_0$ ($j\geqslant 2$) are the parameters characterizing the renormalization scheme, by solving the renormalization group equation (RGE) [26]

$$\frac{da(\mu)}{d\ln\mu^2}=-\beta_0 a^2(\mu)(1+c_1 a(\mu)+c_2 a^2(\mu)+\cdots) \tag{3}$$

$$\Rightarrow\ln\left(\frac{\tilde{\Lambda}^2}{\mu^2}\right)=\frac{1}{\beta_0}\int_0^{a(\mu)}dx\left[\frac{1}{x^2(1+c_1x+c_2x^2+\cdots)}-\frac{1}{x^2(1+c_1x)}\right]-\frac{1}{\beta_0 a(\mu)}+\frac{c_1}{\beta_0}\ln\left(\frac{1+c_1a(\mu)}{c_1a(\mu)}\right) \tag{4}$$

$$\Rightarrow\tilde{\Lambda}=\mu\exp\left(-\frac{1}{2\beta_0 a(\mu)}\right)\left(\frac{1+c_1a(\mu)}{c_1a(\mu)}\right)^{\nu}\times\exp\left[-\frac{1}{2\beta_0}\int_0^{a(\mu)}dx\times\frac{(c_2+c_3x+c_4x^2+\cdots)}{(1+c_1x)(1+c_1x+c_2x^2+\cdots)}\right], \tag{5}$$

where $\nu=c_1/(2\beta_0)=\underline{\beta_1}/(2\beta_0^2)$; the coefficients $c_j$ ($j\geqslant 2$) will be taken here in $\overline{\rm MS}$ scheme. Expansion of expression (5) in powers of $a(\mu)$ then gives

$$\tilde{\Lambda}=\mu\exp\left(-\frac{1}{2\beta_0 a(\mu)}\right)a(\mu)^{-\nu}c_1^{-\nu}\left[1+\sum_{k=1}^{\infty}\tilde{r}_k a^k(\mu)\right], \tag{6}$$

where

$$\tilde{r}_1=\frac{(c_1^2-c_2)}{2\beta_0},$$

$$\tilde{r}_2=\frac{1}{8\beta_0^2}[(c_1^2-c_2)^2-2\beta_0(c_1^3-2c_1c_2+c_3)], \tag{7a}$$

$$\tilde{r}_3=\frac{1}{48\beta_0^3}[(c_1^2-c_2)^3-6\beta_0(c_1^2-c_2)(c_1^3-2c_1c_2+c_3)+8\beta_0^2(c_1^4-3c_1^2c_2+c_2^2+2c_1c_3-c_4)]. \tag{7b}$$

On the other hand, for the uncertainty in $m_q$ from the $b=1/2$ renormalon singularity to be proportional to the quan-

TABLE I. The $\overline{\rm MS}$ RGE coefficients $c_k=\beta_k/\beta_0$ $(k=1,2,3,4)$ and renormalon coefficients $\nu$ and $\tilde{c}_j$ $(j=1,2,3)$ for the $b\bar{b}$ $(n_f=4)$ and $t\bar{t}$ $(n_f=5)$ system.

| $n_f$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $\nu$ | $\tilde{c}_1$ | $\tilde{c}_2$ | $\tilde{c}_3$ |
|---|---|---|---|---|---|---|---|---|
| 4 | 1.5400 | 3.0476 | 15.0660 | $(40\pm 60)$ | 0.3696 | $-0.1054$ | 0.2736 | $(0.01\mp 0.17)$ |
| 5 | 1.2609 | 1.4748 | 9.8349 | $(70\pm 20)$ | 0.3289 | 0.0238 | 0.3265 | $(-0.20\mp 0.08)$ |

tity (6), this implies that the singular part of the Borel transform $B_S(b)$ around $b=1/2$ must have the form[1]

$$B_S(b;\mu)=N_m\pi\frac{\mu}{\overline{m}_q}\frac{1}{(1-2b)^{1+\nu}}\left[1+\sum_{k=1}^{\infty}\tilde{c}_k(1-2b)^k\right]+B_S^{(\rm an.)}(b;\mu), \tag{8a}$$

$$\tilde{c}_1=\frac{\tilde{r}_1}{(2\beta_0)\nu},\quad \tilde{c}_2=\frac{\tilde{r}_2}{(2\beta_0)^2\nu(\nu-1)},$$

$$\tilde{c}_3=\frac{\tilde{r}_3}{(2\beta_0)^3\nu(\nu-1)(\nu-2)}, \tag{8b}$$

and $B_S^{(\rm an.)}(b;\mu)$ is analytic on the disk $|b|<1$. The $\overline{\rm MS}$ coefficients $c_2$ and $c_3$ are already known [28,29], but for $c_4$ we have only estimates [30,31] obtained by Padé-related methods. Reference [30] gives $c_4\approx 97(n_f=4);86(n_f=5)$, and Ref. [31] gives $c_4\approx 40(n_f=4);70(n_f=5)$. However, the estimate of [30] is obtained from a polynomial in $n_f$ with estimated coefficients, where large cancellations occur between various terms. Therefore, we will take as the central values the estimates of [31], with the edges of the $(\pm)$ uncertainties covering the values of [30]

$$c_4=40\pm 60\quad (n_f=4), \tag{9a}$$

$$c_4=70\pm 20\quad (n_f=5). \tag{9b}$$

Thus, $\tilde{c}_3$ can be obtained via Eqs. (7b), (8b): $\tilde{c}_3=0.01\pm 0.17$ $(n_f=4)$; $-0.20\pm 0.08$ $(n_f=5)$. The values of $c_k$'s and $\tilde{c}_k$'s are given in Table I. Now, the (full) bilocal method [18] consists of taking in the expansion (8a) for the analytic part $B_S^{(\rm an.)}$ a polynomial in powers of $b$, so that the expansion of $B_S$ around $b=0$ agrees with expansion (2). For that, the residue parameter $N_m$ in Eq. (8a) has to be determined. Using the idea of Ref. [32] it was estimated with a high precision in Refs. [13,14,33]:

$$N_m=\frac{\overline{m}_q}{\mu}\frac{1}{\pi}R_S(b=1/2), \tag{10}$$

where, according to (8a)

$$R_S(b;\mu)\equiv(1-2b)^{1+\nu}B_S(b;\mu). \tag{11}$$

[1]See, for example, Ref. [22] for some algebraic details of obtaining the typical renormalon ambiguity $\mathrm{Im}\,S(z=2\beta_0 a(\mu)\pm i\varepsilon)$.

In this work, in applications of the bilocal and related methods, we will use the value of $N_m$ as estimated in Ref. [33], which used for $R_S(b)$ truncated perturbation series (TPS) and Padé approximation [1/1]:

$$N_m(n_f=4)=0.555\pm 0.020, \tag{12a}$$

$$N_m(n_f=5)=0.533\pm 0.020. \tag{12b}$$

The bilocal expansion (8a) has then for the analytic part the polynomial

$$B_S^{(\rm an.)}(b;\mu)=h_0^{(m)}+\frac{h_1^{(m)}}{1!\beta_0}b+\frac{h_2^{(m)}}{2!\beta_0^2}b^2, \tag{13a}$$

$$h_k^{(m)}=\frac{4}{3}r_k-\pi N_m\frac{\mu}{\overline{m}_q}(2\beta_0)^k\sum_{n=0}^{3}\tilde{c}_n\frac{\Gamma(\nu+k+1-n)}{\Gamma(\nu+1-n)}, \tag{13b}$$

where, by convention, $r_0=\tilde{c}_0=1$. We can then take for $B_S$ the bilocal formula, i.e., Eqs. (8a) and (13) with the expansion around $b=1/2$ in the singular renormalon part truncated with the term $\tilde{c}_3(1-2b)^3$,

$$B_S(b;\mu)^{(\rm biloc.)}=N_m\pi\frac{\mu}{\overline{m}_q}\frac{1}{(1-2b)^{1+\nu}}\left[1+\sum_{k=1}^{3}\tilde{c}_k(1-2b)^k\right]+\sum_{k=0}^{2}\frac{h_k^{(m)}}{k!\beta_0^k}b^k. \tag{14}$$

Applying the (generalized) principal value (PV) prescription for the Borel integration

$$S=\frac{1}{\beta_0}\mathrm{Re}\int_{\pm i\varepsilon}^{\infty\pm i\varepsilon}db\,\exp\left(-\frac{b}{\beta_0 a(\mu)}\right)B_S(b;\mu), \tag{15}$$

we obtain the pole mass $m_q$ in terms of the mass $\overline{m}_q$. The numerical integration is performed, using the Cauchy theorem, along a ray with a nonzero finite angle with respect to the $b>0$ axis, in order to avoid the vicinity of the pole (as explained, for example, in Ref. [20]).

In Figs. 1(a), (b), we present the resulting (PV) pole masses of the $b$ and $t$ quarks, as function of the renormalization scale $\mu$. The spurious $\mu$-dependence is very weak. In addition, results of another method (''R''-method) are presented in Figs. 1(a), (b), with the $\mu$-dependence stronger in

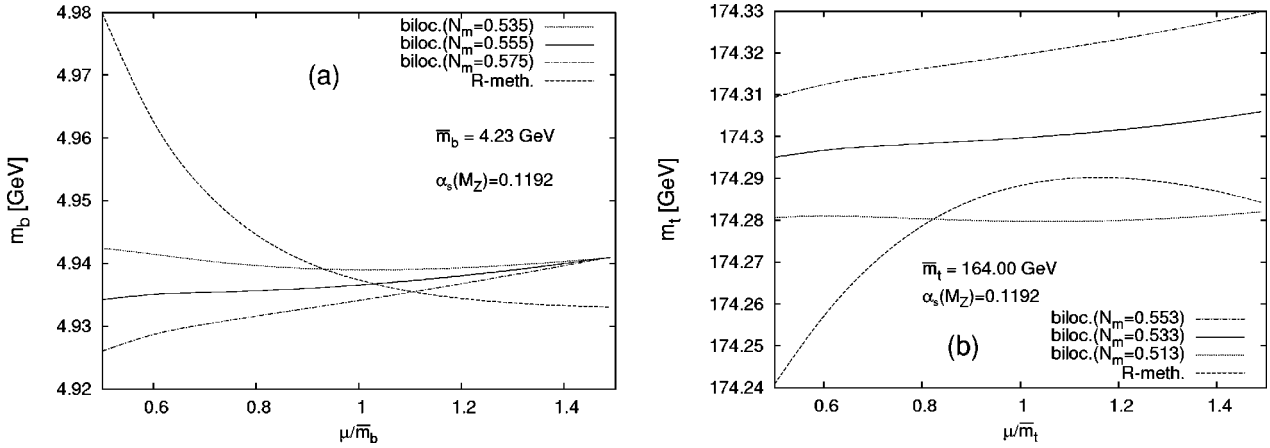


FIG. 1. The (PV) pole mass of the (a) bottom and (b) top quark, as function of the renormalization scale $\mu$. The input parameters used were $\bar{m}_b = 4.23$ GeV, $\bar{m}_t = 164.00$ GeV, respectively; the residue parameter values (12) were used for the bilocal method. The reference value for $\alpha_s$ (in $\overline{\rm MS}$) was taken to be $\alpha_s(m_\tau) = 0.3254$ ( [34]) corresponding to $\alpha_s(M_Z) = 0.1192$.

the low-$\mu$ region ($\mu/\bar{m}_q < 1$). The R-method (applied in other contexts in Refs. [19,20]) consists in the Borel integration of the function (11)

$$S = \frac{1}{\beta_0} \mathrm{Re} \int_{\pm i\varepsilon}^{\infty \pm i\varepsilon} db \exp\left( -\frac{b}{\beta_0 a(\mu)} \right) \frac{R_S(b;\mu)}{(1-2b)^{1+\nu}}, \tag{16}$$

where for $R_S(b)$ the corresponding (NNLO) TPS is used. When we take $\bar{m}_b = 4.23$ GeV and $\bar{m}_t = 164.00$ GeV and we vary the values of the residue parameter $N_m$ according to Eq. (12), the bilocal method gives, at $\mu/\bar{m}_q = 1$, variation $\delta m_b = \mp 3$ MeV and $\delta m_t = \pm 20$ MeV. When the central values of $N_m$ (12) are used, the variation of the obtained values of $m_q$ with $\mu$, when $\mu/\bar{m}_q$ grows from 1.0 to 1.5, is about 5 MeV and 6 MeV for $m_b$ and $m_t$, respectively (for *R*-method: 4 MeV and 6 MeV). When $c_4$ is varied according to (9), the variation is about $\mp 2$ and $\mp 1$ MeV for $m_b$, $m_t$, respectively. The $\alpha_s(m_\tau) = 0.3254 \pm 0.0125$ [34], corresponding to $\alpha_s(M_Z) = 0.1192 \pm 0.0015$. This uncertainty is by far the major source in the variation of the pole masses: $(\delta m_b)_{\alpha_s} = {}^{+135}_{-148}$ MeV for bilocal method ($^{+137}_{-150}$ MeV for *R*-method), and $(\delta m_t)_{\alpha_s} = {}^{+161}_{-171}$ MeV for bilocal method ($^{+161}_{-170}$ MeV for *R*-method).

The natural renormalization scale $\mu$ here is a hard scale $\mu \sim \bar{m}_q$, and will be denoted later in this work as $\mu_m$ in order to distinguish it from the "soft" renormalization scale $\mu$ used in the analogous renormalon-based resummations of the (hard+)soft binding energy $E_{q\bar{q}}(s)$ ($\bar{m}_q > \mu \gtrsim \bar{m}_q \alpha_s$) in Sec. IV. The fact that the two renormalization scales are different does not affect the mechanism of the ($b = 1/2$) renormalon cancellation in the bilocal calculations of the meson mass ($2m_q + E_{q\bar{q}}(s)$), because the renormalon ambiguity in each of the two terms is renormalization scale independent $\sim \tilde{\Lambda}$, as seen by Eqs. (6)–(8). On the other hand, if *R*-type methods (16) [cf. also Eq. (10)] are applied for the resummations of $2m_q$ and $E_{q\bar{q}}(s)$, the renormalon ambiguities are renormalization scale independent in the approximation of the one-loop RGE running, and the renormalon cancellation is true at this one-loop level.

## III. SEPARATION OF THE SOFT AND ULTRASOFT CONTRIBUTIONS

The perturbation expansion of the (hard + soft + ultrasoft) binding energy $E_{q\bar{q}}$ of the $q\bar{q}$ heavy quarkonium vector ($S = 1$) or scalar ($S = 0$) ground state ($n = 1, \ell = 0$) up to the N$^3$LO $\mathcal{O}(m_q \alpha_s^5)$ was given in [35], where previous results of Ref. [3] were used. The latter reference used in part the results of Refs. [2,36–38] (static potential) and of Refs. [39–43] (binding energy). Reference [35] (and [3]) employed the method of threshold expansion where the integrations were performed in $(3 - 2\varepsilon)$ dimensions. The reference mass scale used was the pole mass $m_q$. The ground state energy expansion has the form

$$E_{q\bar{q}} = -\frac{4}{9} m_q \pi^2 a^2(\mu) \{1 + a(\mu)[k_{1,0} + k_{1,1} L_p(\mu)] + a^2(\mu) \times [k_{2,0} + k_{2,1} L_p(\mu) + k_{2,2} L_p^2(\mu)] + a^3(\mu)[k_{3,0} + k_{3,1} L_p(\mu) + k_{3,2} L_p^2(\mu) + k_{3,3} L_p^3(\mu)] + \mathcal{O}(a^4)\}, \tag{17}$$

where

$$L_p(\mu) = \ln\left( \frac{\mu}{\frac{4}{3} m_q \pi a(\mu)} \right). \tag{18}$$

The expressions for the coefficients $k_{i,j}$ of perturbation expansion (17) for the ground state binding energy of the quarkonium ($n = 1$; $\ell = 0$; $S = 1$ or 0) are given below. The NLO and NNLO terms were obtained in Refs. [40–43]. The N$^3$LO terms were obtained in Ref. [35]–their Eqs. (6) and (12), but now written in numerically more explicit form (and with $N_c = 3$),

$$k_{1,1}=4\beta_0,\quad k_{1,0}=\left(\frac{97}{6}-\frac{11}{9}n_f\right), \tag{19a}$$

$$k_{2,2}=12\beta_0^2,\quad k_{2,1}=\frac{927}{4}-\frac{193}{6}n_f+n_f^2, \tag{19b}$$

$$k_{2,0}=361.342-40.9649n_f+1.16286n_f^2-11.6973S(S+1), \tag{19c}$$

$$k_{3,3}=32\beta_0^3,\quad k_{3,2}=\frac{4521}{2}-\frac{10955}{24}n_f+\frac{1027}{36}n_f^2-\frac{5}{9}n_f^3, \tag{19d}$$

$$k_{3,1}=7242.3-1243.95n_f+69.1066n_f^2-1.21714n_f^3+\frac{\pi^2}{2592}(-67584+4096n_f)S(S+1), \tag{19e}$$

$$k_{3,0}=\Bigg[(7839.82-1223.68n_f+69.4508n_f^2-1.21475n_f^3)+(-109.05+4.06858n_f)S(S+1)-\frac{\pi^2}{18}(-1089+112S(S+1))\ln(a(\mu))+2\frac{a_3}{4^3}\Bigg]. \tag{19f}$$

Here, $a_3$ is the hitherto unknown three-loop contribution coefficient to the QCD static potential $V_{q\bar{q}}(r)$, whose values have been estimated by various methods in Refs. [44,13,14,33]. We will use in this work the estimates of Ref. [33], obtained from the condition of renormalon cancellation in the sum $(2m_q+V_{q\bar{q}}(r))$

$$\frac{1}{4^3}a_3(n_f=4)\approx 86\pm 23, \tag{20a}$$

$$\frac{1}{4^3}a_3(n_f=5)=62.5\pm 20. \tag{20b}$$

The coefficients (19) in the expansion (17) originate from quantum effects from various scale regimes of the participating particles: (a) the hard scales ($\sim m_q$); (b) the soft and potential scales where the three momenta are $|\mathbf{q}|\sim m_q\alpha_s$ ($|q^0|\sim m_q\alpha_s$ in the soft and $|q^0|\sim m_q\alpha_s^2$ in the potential regime); (c) ultrasoft scales where $|q^0|$ and $|\mathbf{q}|$ are both $\sim m_q\alpha_s^2$. The coefficients are dominated by the soft scales; the hard scales start contributing at the NNLO [3] and are numerically smaller. For this reason, in this work we will usually refer to the combined soft and hard regime contributions to the binding energy as simply soft ($s$) contribution $E_{q\bar{q}}(s)$. Strictly speaking, it is only the pure soft regime that contributes to the $b=1/2$ renormalon. However, for simplicity, in our renormalon-based resummations we will resum the hard+soft contributions $E_{q\bar{q}}(s)$ together, not separately. This will pose no problem, since the hard regime, being clearly perturbative, is not expected to deteriorate the convergence properties of the series for $E_{q\bar{q}}(s)$. The natural renormalization scale $\mu$ in the resummations of $E_{q\bar{q}}(s)$ is expected to be closer to the soft scale ($m_q\alpha_s\lesssim\mu<m_q$).

On the other hand, the N$^3$LO coefficient $k_{3,0}$ obtains additional contributions from the ultrasoft ($us$) regime. The leading ultrasoft contribution comes from the exchange of an ultrasoft gluon in the heavy quarkonium [5,10]. It consists of two parts:

(1) The retarded part, which cannot be interpreted in terms of an instantaneous interaction

$$\frac{1}{\pi^3}k_{3,0}(us,\text{ret.})=-\frac{2}{3\pi}\left(\frac{4}{3}\right)^2 L_1^E\approx+41.014, \tag{21}$$

where $L_1^E\approx-81.538$ is the QCD Bethe logarithm—see Refs. [3,5].

(2) The non-retarded part can be calculated as expectation value of the $us$ effective Hamiltonian $\mathcal{H}^{us}$ in the Coulomb (i.e., leading order) ground state $|1\rangle$, where $\mathcal{H}^{us}$ (in momentum space) was derived in Refs. [3,5]. Direct calculation of the expectation value, here in coordinate space, then gives:

$$\begin{aligned}\frac{1}{\pi^3}k_{3,0}(us,\text{nonret.})&=-\frac{9}{4\pi^5}\frac{1}{m_q a^5(\mu)}\langle 1|\mathcal{H}^{us}|1\rangle\\&=\frac{2}{\pi^5 m_q a^4(\mu)}\left[\frac{1}{2}\ln\frac{\mu_f^2}{(E_1^C)^2}+\frac{5}{6}-\ln 2\right]\\&\quad\times\Bigg\{-\frac{27\pi^3}{8}a^3(\mu)\langle 1|\frac{1}{r}|1\rangle\\&\quad-17\pi^2\frac{a^2(\mu)}{m_q}\langle 1|\frac{1}{r^2}|1\rangle\\&\quad+\frac{4\pi^2}{3}\frac{a(\mu)}{m_q^2}\langle 1|\delta(\mathbf{r})|1\rangle\\&\quad+3\pi\frac{a(\mu)}{m_q^2}\langle 1|\left\{\Delta_{\mathbf{r}},\frac{1}{r}\right\}|1\rangle\Bigg\}\end{aligned} \tag{22a}$$

$$=-14.196\left[\ln\left(\frac{\mu_f}{m_q\alpha_s^2(\mu)}\right)+0.9511\right]. \tag{22b}$$

Here, $E_1^C=-(4/9)m_q\alpha_s^2(\mu)$ is the Coulomb energy of the state $|1\rangle$, and $\mu_f$ is the factorization energy between the soft ($\sim m_q\alpha_s$) and ultrasoft ($\sim m_q\alpha_s^2$) scale.

In Ref. [3], the authors included in the ultrasoft part of the Hamiltonian additional terms $\delta\mathcal{H}^{us}$ which contained contributions from the soft regime. These terms arose because of their use of a method called threshold expansion [45] where the integrations over potential momenta are not performed in three dimensions but in $(d-1)=(3-2\varepsilon)$ dimensions. However, their method gave in the soft regime also the same additional terms, but with negative sign (including logarithmic terms not associated with IR-divergent integrals–unphysical). Since they were interested in the total sum of

contributions from various regimes, the method gave the correct result, as emphasized by the authors there.

The $s-us$ factorization scale $\mu_f$ can be estimated as being roughly in the middle between the $s$ and $us$ energies on the logarithmic scale [33]

$$\mu_f[\approx (E_S E_{US})^{1/2}] = \kappa m_q \alpha_s(\mu_s)^{3/2}, \tag{23}$$

where $\kappa \sim 1$ and $\mu_s \approx E_S$ ($\lesssim \mu$). Therefore, the ultrasoft part of the N$^3$LO coefficient $k_{3,0}$ can be rewritten, by Eqs. (21), (22) and (23), in terms of the $s-us$ parameter $\kappa$ as

$$\frac{1}{\pi^3} k_{3,0}(us) = 27.512 + 7.098 \ln(\alpha_s(\mu_s)) - 14.196 \ln(\kappa). \tag{24}$$

The soft scale $\mu_s$ appearing here will be fixed by the condition $\mu_s = (4/3)\overline{m}_q \alpha_s(\mu_s)$.

The formal perturbation expansions for the separate soft and ultrasoft parts of the ground state binding energy (17) are then

$$E_{q\bar{q}}(s) = -\frac{4}{9} m_q \pi^2 a^2(\mu) \Bigg\{ 1 + \sum_{i=1}^{2} a^i(\mu) \sum_{j=0}^{i} k_{i,j} L_p(\mu)^j + a^3(\mu) \sum_{j=1}^{3} k_{3,j} + a^3(\mu)[k_{3,0} - k_{3,0}(us)] + \mathcal{O}(a^4) \Bigg\}, \tag{25a}$$

$$E_{q\bar{q}}(us) = -\frac{4}{9} m_q \pi^2 a^2(\mu) \{ a^3(\mu) k_{3,0}(us) + \mathcal{O}(a^4) \}. \tag{25b}$$

The energy $E_{q\bar{q}}(s)$ (25a) contains the leading IR renormalon effects, and $E_{q\bar{q}}(us)$ (25b) does not. In these expressions, the common factor is the soft scale $\mu_p(\mu) = (4/3) m_q \alpha_s(\mu)$ which is also present as the reference scale in the logarithms $L_p(\mu) = \ln(\mu/\mu_p(\mu))$ appearing with the coefficients $k_{i,j}$ (when $j \geqslant 1$) in Eqs. (17), (18). This soft scale is equal to $2/a_B(\mu)$ where $a_B$ is the (Bohr) radius of the heavy quarkonium. The renormalization scale $\mu$ in Eq. (25a) is of the order of the soft scale or above. We will re-express $m_q$ everywhere in $E_{q\bar{q}}$ with the renormalon-free mass $\overline{m}_q$ (1), and will consider the dimensionless soft-energy quantity $E_{q\bar{q}}(s)/\overline{m}_q$.

The expansion of $E_{q\bar{q}}(s)/\overline{m}_q = \Sigma_0^\infty \tilde{r}_n(\mu) a^{n+2}(\mu)$ has at large orders the seemingly peculiar feature of the so-called "power mismatch" [16] (see also [46]): when this sum is added to the expansion (1) $2m_q/\overline{m}_q = [2 + (8/3)\Sigma_0^\infty r_n(\mu) a^{n+1}(\mu)]$, the coefficient $\tilde{r}_n(\mu)$ at powers $a^{n+2}(\mu)$ of $E_{q\bar{q}}(s)/\overline{m}_q$ must be combined with the coefficient $(8/3) r_n(\mu)$ at powers $a^{n+1}(\mu)$ of $2m_q/\overline{m}_q$ to ensure the cancellation of the $b = 1/2$ renormalon contributions. This is so because the coefficient $\tilde{r}_n(\mu)$ contains a polynomial of $n$th grade in $\ln[\mu/(\overline{m}_q a(\mu))]$ [cf. Eqs. (17), (18), (25a)] which, at large order $n$ and in the large-$\beta_0$ approximation, sums up approximately to a term $\sim (\beta_0/2)^n n! \exp \ln[\mu/(\overline{m}_q a(\mu))] = (\beta_0/2)^n n! (\mu/\overline{m}_q) 1/a(\mu)$ [16], effectively reducing the power of $a(\mu)$ in $E_{q\bar{q}}(s)/\overline{m}_q$ by one. Further, the factors $(\beta_0/2)^n$, $n!$ and $\mu$ in the approximate sum of the logarithmic terms in $\tilde{r}_n(\mu)$ reflect the effect of the leading ($b = 1/2$) IR renormalon in $E_{q\bar{q}}(s)/\overline{m}_q$.

For the Borel-related resummations of $E_{q\bar{q}}(s)$, which would account for the leading IR renormalon structure, we have on the basis of these facts in principle at least two possible directions to proceed. The first direction would be to use the Borel transform of the expansion of $E_{q\bar{q}}(s)/\overline{m}_q = \Sigma_0^\infty \tilde{r}_n(\mu) a^{n+2}(\mu)$ where the transformation $a(\mu) \mapsto b$ is performed literally with respect to all $a(\mu)$-dependence, including the one appearing in the coefficients $\tilde{r}_n$. This would result in a Borel transform whose power expansion around the origin would include terms $b^k \ln^\ell b$ with $\ell = 0,1,2,\ldots$.

The second direction would be to divide the considered quantity by $a(\tilde{\mu})$ ($\Rightarrow E_{q\bar{q}}(s)/[\overline{m}_q a(\tilde{\mu})]$), where $\tilde{\mu}$ is any fixed soft scale, and then consider the coefficients in the expansion of this quantity in powers of $a(\mu)$ as independent of $a(\mu)$, e.g., by expressing them in terms of $a(\tilde{\mu})$. In the obtained expansion, the coefficients now contain powers of logarithms $\ln[a(\tilde{\mu})]$ which are considered as constant (nonvariable) under the Borel transformation $a(\mu) \mapsto b$.[2] It is possible to see that, at large $n$ and in the large-$\beta_0$ approximation, this is equivalent to the first approach, because the powers of $a(\mu)$ have been decreased by one, and the coefficients are now proportional to $(\beta_0/2)^n n! \mu/a(\tilde{\mu})$ where the factor $1/a(\tilde{\mu})$ is now formally constant and does not affect the Borel transform (except as an overall constant factor). The equivalence is assumed to persist when we go beyond the large-$\beta_0$ approximation, in the same spirit as the authors of Ref. [16] assume their conclusions to be valid beyond large-$\beta_0$.

We stress that in both approaches the original expansion of $E_{q\bar{q}}(s)$ in powers of $a(\mu)$ is recovered by applying the Borel integration according to the standard formula (15) term-by-term to the expansion of the Borel transform around $b = 0$.

In this work, we decide to follow the second direction. The main reason for this is of practical nature: The first approach would generate in the expansion of the Borel transform around $b = 0$ the terms containing $\ln b, \ln^2 b, \ldots$, which introduce, at any finite order at least, a cut-singularity along the entire negative axis in the $b$ plane. We are working at finite orders. This cut would seriously hamper our resummations. For example, the quantity analogous to $R_S(b)$ Eq. (11) of the previous section, but this time for $E_{q\bar{q}}(s)/\overline{m}_q$

[2]This is in close analogy with the behavior of the static potential $V_{q\bar{q}}(r)$ and its dimensionless version $rV_{q\bar{q}}(r)$ where $r \sim a_B \sim 1/[\overline{m}_q a(\tilde{\mu})]$ (see, for example, Refs. [9–11,13,14,33]).

with the first approach, has a cut along $b \leqslant 0$, i.e., starting already at the origin, and the resummation at $b=1/2$ would be difficult. On the other hand, the analogous quantity $R(b)$ for $E_{q\bar{q}}(s)/[\overline{m}_q a(\tilde{\mu})]$ in the second approach has no singularities at $|b|<1/2$, and for $1/2 \leqslant |b|<1$ has only a cut without infinity along the positive axis. Such a quantity can be much more easily resummed on the basis of its expansion around $b=0$. Nonetheless, the first approach presents an interesting alternative for which resummation techniques other than those presented here would have to be developed and/or applied.

Thus, we will divide the soft binding energy with the quantity $\overline{\mu}(\tilde{\mu})=(4/3)\overline{m}_q \alpha_s(\tilde{\mu})$, where $\tilde{\mu}$ can be any soft scale. We will fix this scale by the condition $\tilde{\mu}=(4/3)\overline{m}_q \alpha_s(\tilde{\mu})$ $(\Rightarrow \tilde{\mu}=\mu_s)$. Further, in the logarithms $L_p(\mu)$ we express the pole mass $m_q$ in terms of $\overline{m}_q$ and powers of $a(\mu)$ (cf. Sec. II), and the powers of logarithms $\ln^k[a(\mu)]$ we re-express in terms of $\ln^k[a(\tilde{\mu})]$. This then results in the following soft binding energy quantity $F(s)$ to be resummed:

$$F(s) \equiv -\frac{9}{4\pi^2}\frac{E_{q\bar{q}}(s)}{\overline{m}_q a(\tilde{\mu})} = a(\mu)[1+a(\mu)f_1+a^2(\mu)f_2 + a^3(\mu)f_3+\mathcal{O}(a^4)], \tag{26}$$

where the coefficients $f_j$ depend on $\ln a(\tilde{\mu})$ and on three scales: the renormalization scale $\mu$ $(\gtrsim m_q \alpha_s)$, the (fixed) soft scale $\tilde{\mu}$, and $\overline{m}_q$. The coefficient $f_3$ depends, in addition, on the parameters $\kappa$ (23)–(24), $\mu_s$, and $a_3$ (20). The coefficients $f_j$ are written explicitly in the Appendix. The $b=1/2$ renormalon in the quantity $F(s)$ is then of the type of the renormalon of the pole mass $m_q$ discussed in the previous Sec. II.

However, if we divided in Eq. (26) by $m_q$ instead of $\overline{m}_q$ and at the same time used in the resulting $f_j$-coefficients $\ln m_q$, the numerical resummations of $F(s)$ by methods of Sec. IV would give us values for $E_{q\bar{q}}(s)$ different usually by not more than $\mathcal{O}(10^1$ MeV) (we checked this numerically). We will briefly refer to these approaches later in this section as ''pole mass'' approaches. A version of such pole mass bilocal approach was applied in Ref. [14] for resummation of the unseparated $E_{q\bar{q}}(s+us)$.

The ultrasoft part (25b), on the other hand, has no $b=1/2$ renormalon. The mass scale used there should also be renormalon free $(\overline{m}_q)$. The renormalization scale $\mu$ there should be adjusted downward to the typical *us* scale of the associated process $\mu \mapsto \mu_{us}$ $(\sim m_q \alpha_s^2)$ in order to come closer to a realistic estimate[3]

$$E_{q\bar{q}}(us) \approx -\frac{4}{9}\overline{m}_q \pi^2 k_{3,0}(us) a^5(\mu_{us}). \tag{27}$$

## IV. EVALUATION OF THE BINDING ENERGY

In this section we will evaluate the soft part of the ground state energy for the vector $b\bar{b}$ $[\Upsilon(1S)]$ and for the vector and scalar $t\bar{t}$ quarkonium. In addition, we will estimate the ultrasoft part of the energy, and will extract the value of the mass $\overline{m}_b$ from the known mass of $\Upsilon(1S)$.

### A. Methods of resummation for the soft energy

At first we will apply the same methods as those used in Sec. II. However, the expansion we will use for the soft energy quantity $F(s)$ (26) is higher by one order in $a(\mu)$ than in quantity $S$ Eq. (1) of Sec. II. In the N$^3$LO coefficient $f_3$ we have dependence on the approximately known coefficient $a_3$ (20), and on the *s-us* factorization scale parameter $\kappa \sim 1$ Eq. (23)—see the Appendix, Eqs. (A4). It turns out that, in $f_3$ $(f_3^{(0)})$, the coefficient at $\ln \kappa$ is larger than the coefficient at $a_3/(100\times 4^3)$. On the other hand, the coefficient at $\ln \kappa$ in the ground state expectation value of the static potential is about one tenth of the corresponding coefficient in the (soft) ground binding energy

$$E_{q\bar{q}}(s;\ln\kappa-\text{part}) \approx -1.93\times 10^3 (\overline{m}_q a^4(\mu))\ln\kappa, \tag{28a}$$

$$\langle 1|V_{q\bar{q}}(r)|1\rangle(\ln\kappa-\text{part}) \approx -1.95\times 10^2 (\overline{m}_q a^4(\mu))\ln\kappa, \tag{28b}$$

$$E_{q\bar{q}}(s;a_3-\text{part}) = \langle 1|V_{q\bar{q}}(r)|1\rangle(a_3-\text{part}) \approx -8.77\times 10^2 (\overline{m}_q a^4(\mu)) \times \frac{a_3}{100\times 4^3}. \tag{28c}$$

Since $a_3/(100\times 4^3)$ is roughly between zero and one [cf. Eq. (20)], as is also $\ln\kappa$, Eq. (28) shows that the static potential is more influenced by the values of $a_3$ than by $\ln\kappa$, while the situation with the (soft) binding energy is just reversed. More specifically: (a) the static potential is more appropriate to obtain approximate values of $a_3$, as was done, e.g., in Ref. [33] and given in Eq. (20); (b) the soft part of the binding energy $E_{q\bar{q}}(s)$ is more appropriate to obtain approximate values of the *s-us* factorization scale parameter $\kappa$. We recall that in [33], the values of $a_3$ (20) were obtained by requiring that the known values of the renormalon residue parameter $N_m$ (12) be reproduced from the Borel transform of the static potential function $rV_{q\bar{q}}(r)$. Here we will proceed analogously, and will obtain approximate values of $\kappa$ (23) by requiring that the residue parameter values (12) be reproduced from the Borel transform of the soft binding energy quantity $F(s)$ of Eq. (26).

As already mentioned, in contrast to the situation in Sec. II, the coefficients $f_j$ of the perturbation series (26) have

[3]The authors of Ref. [47] employed a somewhat similar idea of using different evaluation methods for contributions to the spectra of heavy quarkonia from different regimes (short, intermediate and long-distance). A similar reasoning was employed, in the context of high-$T$ QCD, in Ref. [48].

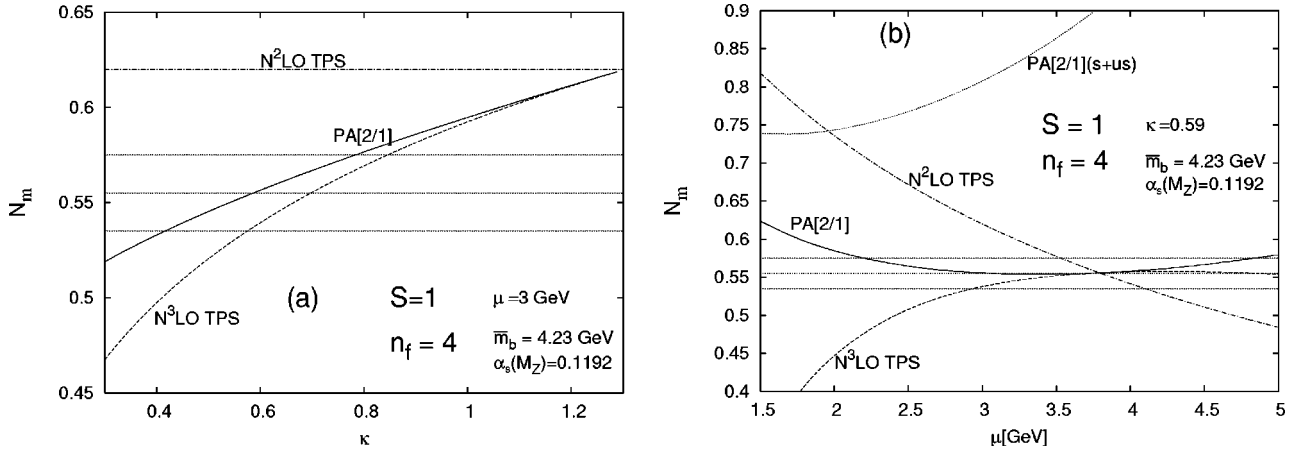


FIG. 2. The residue parameter value $N_m$ as calculated from the soft part of the binding energy of the bottonium according to Eq. (31), (a) as a function of the *s-us* factorization scale parameter $\kappa$ (23), at $\mu=3$ GeV; (b) as a function of the renormalization scale $\mu$, at $\kappa=0.59$. Further explanations given in the text. In (a), the known values (12a) of $N_m$ are denoted as dotted horizontal lines.

some terms proportional to $\ln^k(a(\mu_*))(k=1,2,\ldots)$ where $\mu_*$ generically denotes fixed chosen scales $\tilde{\mu}$, or $\mu_s$—cf. the Appendix. Here we will argue that these scales should be between hard and ultrasoft. These terms are considered constant, independent of $a(\mu)$, although they can be formally re-expressed in terms of $\ln^k a(\mu)$. The terms of the type $\ln a$ in the problem at hand are the leading terms of logarithms of ratios of various scales appearing in the problem (cf. Ref. [3]), among them $\ln(E_S/E_H)$ and $\ln(E_{US}/E_S)$. The typical hard, soft, and ultrasoft scales of the problem are, e.g., $E_H=m_q$, $E_S=\langle 1/r\rangle$, $E_{US}=E_{q\bar{q}}$, i.e., quantities independent of the renormalization scale $(\mu)$.[4] The $\mu$-independent ratios of the type $E_S/E_H$ and $E_{US}/E_S$ have expansions $E_X/E_Y=a(\mu)[1+\mathcal{O}(a)]$. The typical resummed value of this quantity can be written as $a(\mu_*)$ where $\mu_*$ is the typical scale of the quasiobservable $E_X/E_Y$. This suggests that the $\ln a(\mu_*)$-terms in the coefficients of the perturbation series should really be somewhere between hard $(E_H\sim m_q)$ and ultrasoft $(E_{US}\sim m_q\alpha_s^2)$ scales.

Similarly as in Eq. (8a), we have

$$B_{F(s)}(b;\mu)=N_m\frac{9}{2\pi}\frac{\mu}{\overline{m}_q a(\tilde{\mu})}\frac{1}{(1-2b)^{1+\nu}}\times\left[1+\sum_{k=1}^{\infty}\tilde{c}_k(1-2b)^k\right]+B^{(\mathrm{an.})}_{F(s)}(b;\mu), \tag{29}$$

where the factor in front of the singular part was determined by the condition of renormalon cancellation of the sum $2m_q+E_{q\bar{q}}(s)$. We now define in analogy with Eq. (11)

$$R_{F(s)}(b;\mu;\mu_f)=(1-2b)^{1+\nu}B_{F(s)}(b;\mu;\mu_f). \tag{30}$$

Here we denoted, for clarity, explicitly the dependence on the factorization scale $\mu_f$. Expressions (29) and (30) imply

$$N_m=\frac{2\pi}{9}\frac{\overline{m}_q a(\tilde{\mu})}{\mu}R_{F(s)}(b;\mu;\mu_f)|_{b=1/2}. \tag{31}$$

The expansion of $R_{F(s)}$ is exactly known up to $\sim b^2$, and approximately up to $\sim b^3$ ($N^3$LO TPS), where the latter coefficient is dependent on $\kappa$ (and, more weakly, on $a_3$). All coefficients are dependent also on the renormalization scale $\mu$ $(\gtrsim m_q\alpha_s)$. It turns out that the expansion (31) is significantly less convergent than the series (11) (at $b=1/2$). However, it is not clearly divergent, unless we take unreasonable values of $\kappa$ or $\mu$. Theoretically, $R_{F(s)}(b)$ should be a function with only a weak singularity (cut) at $b=1/2$, and the nearest pole at $b=3/2$ (i.e., the next renormalon pole of $V_{q\bar{q}}(r)$ [50]). Thus, resummations such as Padé approximations (PA's) are expected to work better on $R_{F(s)}(b)$ than on $B_{F(s)}(b)$. The Padé approximation with the simplest pole structure for the $N^3$LO TPS is [2/1], i.e., ratio of a quadratic with a linear polynomial in $b$. It turns out that $R_{F(s)}[2/1]\times(b)$ has physically acceptable pole structure $|b_{\mathrm{pole}}|\geqslant 1$ for most of the values of $\mu\gtrsim m_q\alpha_s$ and $\kappa\sim 1$. Using this Padé to evaluate expression (31) gives us predictions for the residue parameter $N_m$ reasonably stable under the variation of $\mu$. On the other hand, the predicted value of $N_m$ depends significantly on the *s-us* factorization scale parameter $\kappa$ (23).

In Fig. 2(a) we show the dependence of $N_m$ on $\kappa$, at a typical (''central'') $\mu$ value $\mu=3$ GeV, for the $b\bar{b}$ system. The known central value (12a) of $N_m$ is obtained by the $R_{F(s)}[2/1](b=1/2)$ expression at $\kappa\approx 0.59$. In Fig. 2(b) we present, for $\kappa=0.59$, the dependence of calculated $N_m$ on the renormalization scale $\mu$. There, we include also the ([2/1]-resummed) curve for the case when no separation of the *s* and *us* parts of the energy is performed. In that case, the obtained values of $N_m$ are unacceptable. If the ''pole mass'' version is applied [mentioned in the second paragraph after Eq. (26)], with no separation of the *s* and *us* parts, the obtained values of the ([2/1]-resummed) curve remain above

[4]A very similar phenomenon occurs in the perturbation expansion of the free energy of the high-temperature quark-gluon plasma, where the hard scale is the Matsubara frequency $2\pi T$, and the soft scale is the Debye screening mass $m_E$ $(\sim g_s T)$ [48,49].

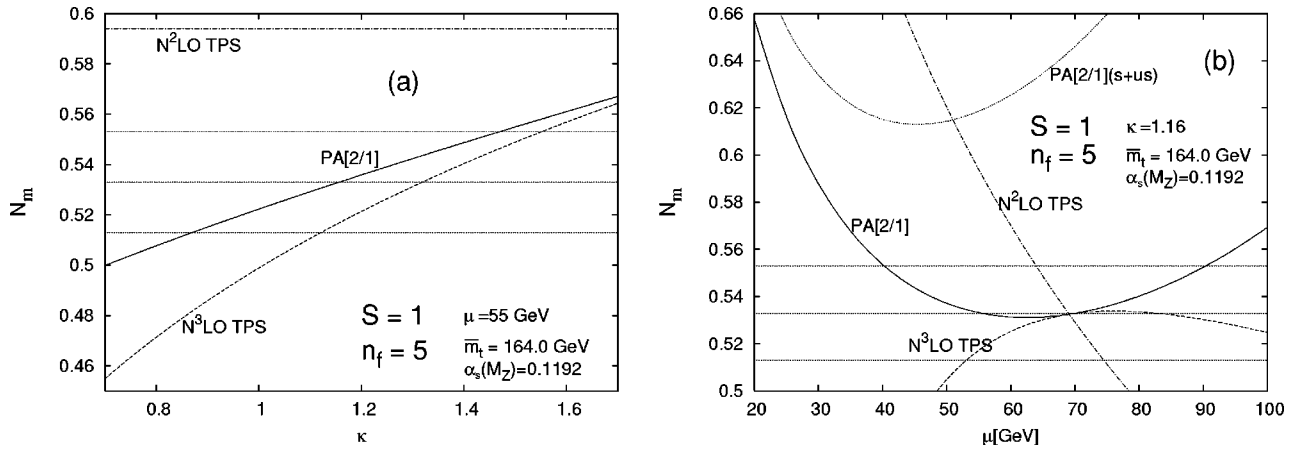


FIG. 3. Same as in Fig. 2, but for the ($S=1$) toponium. In (a), $\mu=55$ GeV and the known values (12b) of $N_m$ are given as dotted horizontal lines.

0.70 as well, thus unacceptable. The other values of the input parameters are chosen to have the $b\bar{b}$ "central" values: $a_3/4^3=86$ (20a); $\bar{m}_b=4.23$ GeV; $\tilde{\mu}=1.825$ GeV ($\approx\mu_s$) and $\alpha_s(\tilde{\mu};n_f=4)=0.3263(\approx\alpha_s(\mu_s;n_f=4)=0.326)$ [from: $\alpha_s(m_\tau;n_f=3)=0.3254$, i.e., $\alpha_s(M_Z)=0.1192$ [34]]. For the RGE running, we always use four-loop $\overline{\rm MS}$ $\beta$-function (TPS) and three-loop quark threshold matching relations [51], with $\mu_{\rm thresh.}=2\bar{m}_c,\ 2\bar{m}_b$.

In Figs. 3 and 4 we present analogous results for the $t\bar{t}$ vector ($S=1$) and scalar ($S=0$) bound state. The typical ("central") values of the renormalization scale were chosen to be $\mu=55$ GeV and 65 GeV, respectively. The *s-us* factorization parameter $\kappa$ values obtained were $\kappa=1.16$ ($S=1$) and $\kappa=1.10$ ($S=0$), so that $R_{F(s)}[2/1](b=1/2)$ would reproduce the known central value (12b) of the residue parameter $N_m$. The other input parameters have the $t\bar{t}$ "central" values: $a_3/4^3=62.5$ (20b); $\bar{m}_t=164.0$ GeV; $\tilde{\mu}=31.$ GeV ($\approx\mu_s$) and $\alpha_s(\tilde{\mu};n_f=5)=0.1430$ [$\approx\alpha_s(\mu_s;n_f=5)=0.14$]. The values of $N_m$ extracted when no separation of *s* and *us* is performed, are unacceptably high $N_m\geqslant 0.6$ (also in the "pole mass" version: $N_m\geqslant 0.6$).

Variation $N_m=0.555\pm0.020$ [$b\bar{b}$, Eq. (12a)] implies $\kappa=0.59\pm0.19$; variation $N_m=0.533\pm0.020$ [$t\bar{t}$, Eq. (12b)] implies $\kappa=1.16^{+0.31}_{-0.29}$ ($S=1$) and $\kappa=1.10^{+0.39}_{-0.33}$ ($S=0$). If, on the other hand, $a_3$ parameter is varied, according to Eq. (20), then for $b\bar{b}$ $\kappa=0.59\mp0.06$, and for $t\bar{t}$ $\kappa=1.16^{-0.10}_{+0.11}$ ($S=1$) and $\kappa=1.10^{-0.09}_{+0.11}$ ($S=0$). Thus, the value of *s-us* factorization scale parameter $\kappa$ is influenced largely by the allowed values (12) of the renormalon residue parameter, and significantly less by the allowed values $a_3$ (20) of the N$^3$LO coefficient of the static $q\bar{q}$ potential. Therefore, we will consider the variations of $N_m$ (12) and of $\kappa$ to be related by a one-to-one relation, while the variations of $a_3$ (20) will be considered as independent.

In this way, we have the following values for the *s-us* factorization scale parameter: $\kappa$ (23)

$$N_m=0.555\pm0.020\Rightarrow\kappa=0.59\pm0.19\quad(n_f=4,S=1), \tag{32a}$$

$$N_m=0.533\pm0.020\Rightarrow\kappa=1.16^{+0.31}_{-0.29}\quad(n_f=5,S=1) \tag{32b}$$

$$\Rightarrow\kappa=1.10^{+0.39}_{-0.33}\quad(n_f=5,S=0), \tag{32c}$$

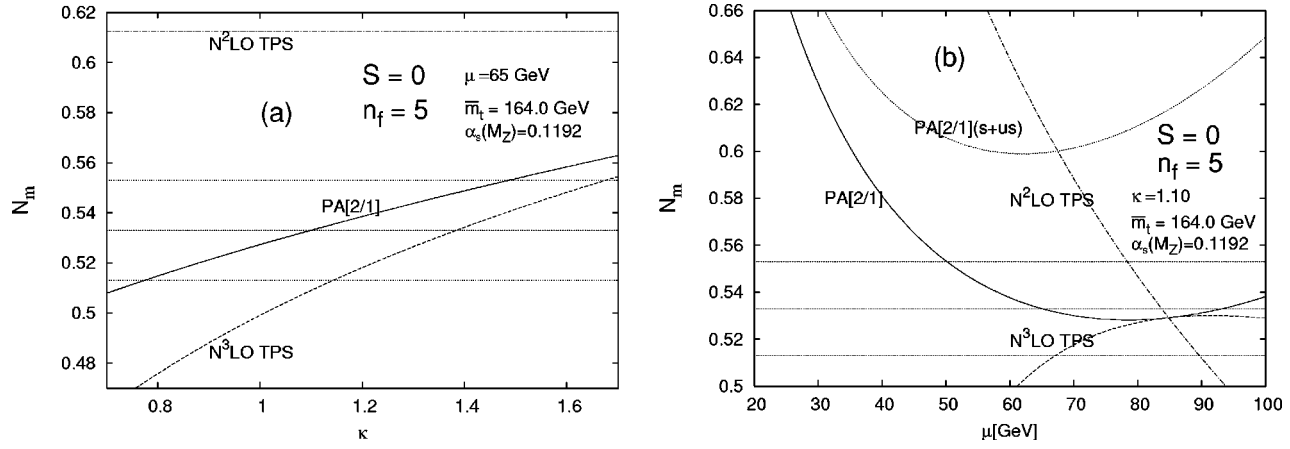


FIG. 4. Same as in Fig. 3, but for the scalar ($S=0$) toponium. In (a), $\mu=65$ GeV is taken.

and thus we obtain the N$^3$LO TPS (26) for the soft part of the ground binding energy.

We wish to add a comment on $\kappa$-dependence of $N_m$ in Figs. 2–4. Theoretically, the parameter $N_m$ should be independent of the *s-us* factorization scale $\mu_f$ and thus independent of the related parameter $\kappa$ (23). However, among the $\mu_f$-dependent terms in $R_{F(s)}(b;\mu;\mu_f)$ of Eq. (30), only the leading term is available. Due to this restrictive practical situation, the value of the residue parameter $N_m$ obtained by Eq. (31) automatically possesses significant $\mu_f$-dependence (or $\kappa$-dependence), and the value of $\mu_f$ (or $\kappa$) is fixed by requiring that this leading order expression in $\mu_f$ reproduces the known value of $N_m$. The value of $\mu_f$ obtained in this way must be physically acceptable ($\Leftrightarrow \kappa \sim 1$) if the procedure is consistent. This is analogous to the situation when a QCD observable $S(Q)$ is known to the leading order $\sim a(\mu)$ only. Equating such leading order expression $S_{[1]}(Q;\mu)$ with the known value of $S(Q)$, a specific value of the renormalization scale $\mu=\mu_{\rm ECH}$ is obtained such that $S_{[1]}(Q;\mu_{\rm ECH})=S(Q)$. This is the main idea of the effective charge (ECH) method [52]. If the procedure is consistent, the obtained renormalization scale $\mu$ value $\mu_{\rm ECH}$ should be of the order of the physical scale $Q$ of the process associated with the observable: $\mu_{\rm ECH}/Q \sim 1$. The analogy with our case consists in the correspondence $\mu_f \leftrightarrow \mu$, $E_{\rm US}(\sim E_{q\bar{q}}) \leftrightarrow Q$, and $\mu_f({\rm obtained}) \leftrightarrow \mu_{\rm ECH}$.

Now that the value of $\kappa$ has been obtained, and consequently the N$^3$LO TPS (26), we can perform the resummation of the soft part of the ground binding energy. The full bilocal method [14,18] can be performed as in Sec. II, Eqs. (14) and (15). However, now we have one term more in the TPS. Therefore

$$B^{({\rm biloc.})}_{F(s)}(b;\mu)=N_m \frac{9}{2\pi}\frac{\mu}{\overline{m}_q a(\tilde{\mu})}\frac{1}{(1-2b)^{1+\nu}} \times \sum_{k=0}^{3}\tilde{c}_k(1-2b)^k+\sum_{k=0}^{3}\frac{h_k}{k!\beta_0^k}b^k, \quad (33)$$

where the coefficients $\tilde{c}_k$ are given by Eqs. (8b) and (7) ($\tilde{c}_0=1$), and the coefficients $h_k$ in the expansion of the analytic part are now known up to order $k=3$,

$$h_k=f_k-N_m\frac{9}{2\pi}\frac{\mu}{\overline{m}_q a(\tilde{\mu})}(2\beta_0)^k\sum_{n=0}^{3}\tilde{c}_n\frac{\Gamma(\nu+k+1-n)}{\Gamma(\nu+1-n)} \quad (k=0,1,2,3). \quad (34)$$

Here, by convention, $f_0=1=\tilde{c}_0$. Then the resummed quantity is obtained by taking the PV of the Borel integration of $B_{F(s)}(b)$ of Eq. (33), as in Sec. II for $B_S(b)$ [Eq. (15), integration along a ray]. The result would have some spurious $\mu$-dependence. However, for the typical $\mu$-scales $m_q \gtrsim \mu \gtrsim m_q\alpha_s$, the analytic part $B^{(\rm an.)}_{F(s)}(b)$ of the Borel transformation in Eq. (33) turns out to have a problematic behavior in the following sense. When it is Padé-resummed as $B^{(\rm an.)}_{F(s)}[2/1](b)$, the obtained pole is almost always (for most $\mu$'s) unacceptably small in size: $|b_{\rm pole}| \leqslant 1/2$. Theoretically, $B^{(\rm an.)}_{F(s)}(b)$ should have the nearest pole at $b=3/2$ [50]. Thus, $B^{(\rm an.)}_{F(s)}$ appears to be too singular in the above bilocal approach, and the TPS and Padé evaluations of it would result in widely differing resummed values for the energy $E_{q\bar{q}}(s)$. The reason for this problem appears to lie in the specific truncated form of the singular part taken in the bilocal method (33). While the latter part describes well the behavior of the transform near $b=1/2$, it influences apparently strongly the coefficients $h_k$ and thus the analytic part, so that no reliable resummation of that part (apart from TPS) can be done. In this context, we note that the series of terms $\Sigma_k \tilde{c}_k(1-2b)^k$ has no indication of convergence at $b=0$, as seen from the values of $\tilde{c}_j$ in Table I of Sec. II. This problem can be alleviated by introducing in the renormalon part a "form" factor which suppresses that part away from $b \approx 1/2$, but keeps it unchanged at $b \approx 1/2$. If we choose for this factor a Gaussian type of function, we are led to the following set of "$\sigma$-regularized" bilocal expressions for the Borel transform:

$$B^{(\sigma)}_{F(s)}(b;\mu)=N_m\frac{9}{2\pi}\frac{\mu}{\overline{m}_q a(\tilde{\mu})}\frac{1}{(1-2b)^{1+\nu}}\Bigg[1+\tilde{c}_1(1-2b)+\left(\tilde{c}_2+\frac{1}{8\sigma^2}\right)(1-2b)^2+\left(\tilde{c}_3+\frac{\tilde{c}_1}{8\sigma^2}\right)(1-2b)^3\Bigg]\exp\left[-\frac{1}{8\sigma^2}(1-2b)^2\right]+\sum_{k=0}^{3}\frac{1}{k!\beta_0^k}h_k^{(\sigma)}b^k. \quad (35)$$

The corrective terms $1/(8\sigma^2)$ and $\tilde{c}_1/(8\sigma^2)$ in the coefficients of the renormalon part of Eq. (35) appear to ensure the correct known behavior of the renormalon part up to order $\sim(1-2b)^{-\nu+2}$. The coefficients $h_k^{(\sigma)}$ in Eq. (35) differ from $h_k$'s of the bilocal case (34), and are determined by the requirement that the power expansion of expression (35) reproduces the known N$^3$LO TPS of the Borel transform of $F_s$ (26). If $\sigma$ parameter increases (i.e., $\sigma \gtrsim 1$), formula (35) is expected to gradually reduce to the bilocal formula (33). If $\sigma \to 0$, then the expansion of the Gaussian form function in (35) would imply very large coefficients ($\gtrsim \sigma^{-4}$) at the renormalon terms $\sim(1-2b)^{-1-\nu+k}$ ($k=4,5,\ldots$). This is not expected to reflect the reality, because the results in Table I suggest that $|\tilde{c}_k| \lesssim 1$ for $k=4,5,\ldots$. Therefore, we expect that the optimal choice of $\sigma$ would be somewhere between zero and one. Numerical analysis confirms this expectation. Namely, when $\sigma$ decreases from $\sigma=\infty$ to about $\sigma \approx 0.3$–$0.4$, the value of the pole of the [2/1] Padé-resummed analytic part $B^{(\rm an.\sigma)}_{F(s)}(b)$ of Eq. (35) gradually turns acceptable ($|b_{\rm pole}|>1$) and rather stable when the renormalization scale $\mu$ varies in the interval $[m_q\alpha_s, m_q]$ (except close to $\mu \approx m_q\alpha_s$). Further, the Borel resummation with the TPS-evaluated and with Padé-evaluated analytic parts give for

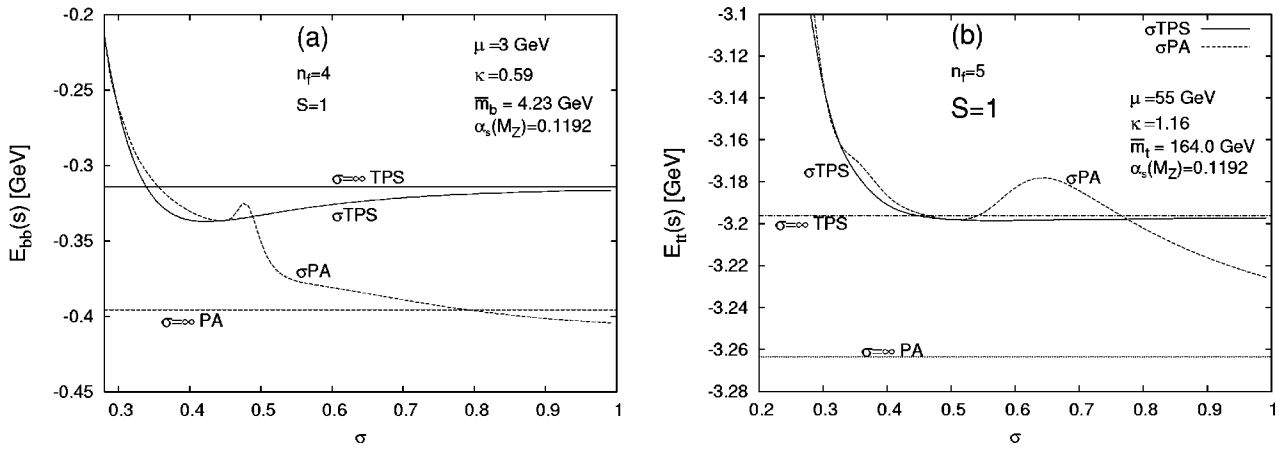


FIG. 5. (a) Soft part of the ground state binding energy of $b\bar{b}$, evaluated with the (PV) Borel-resummed expression (35), as a function of the method parameter $\sigma$. (b) Same as in (a), but for the toponium $S=1$ system. Details are given in the text.

such $\sigma$'s similar values of $E_{q\bar{q}}(s)$, indicating that the analytic part now manifests more clearly its non-singular behavior. When the value of $\sigma$ falls below 0.3, the analytic part starts showing erratic behavior again and the Borel resummation gives significantly differing results with the TPS- and the Padé-evaluated analytic parts. Further, the $\sigma-$dependence of the obtained soft energy becomes very strong for $\sigma<0.3$. On these grounds, the obtained optimal $\sigma$ turn out to be

$$\sigma=0.36\pm0.03 \quad (n_f=4,S=1), \tag{36a}$$

$$\sigma=0.33\pm0.03 \quad (n_f=5,S=0,1). \tag{36b}$$

In Fig. 5(a) we present the (PV) Borel-resummed soft part of ground state energy for the bottonium ($S=1$), as a function of the $\sigma$ parameter of method (35). The results are given when the analytic part of Borel transform (35) is either evaluated as N$^3$LO TPS or as [2/1] Padé (PA). In addition, the two corresponding results (TPS, and PA) are given as horizontal lines when the bilocal method (33) is applied ($\sigma=\infty$). The values of the other input parameters have the same "central" values as in Fig. 2, and $N_m=0.555$ and $c_4=40.$ in accordance with Eqs. (12a) and (9a). In Fig. 5(b) we present analogous results for the toponium vector ($S=1$) soft binding energy. The values of the input parameters are the same as in Figs. 3 and 4, and in addition $N_m=0.533$ and $c_4=70$ in accordance with Eqs. (12b) and (9b). The corresponding curves for the toponium scalar ($S=0$) case are very similar to those of the $S=1$ case.

In addition to the methods (33) and (35) employed up to now, which are mutually related, we want to employ as a cross check of our numerical results also a method unrelated to the (full) bilocal method. This will be the $R$-method [19,20], where we resum the function $R_{F(s)}(b;\mu)$ (30) and then employ the (PV) Borel resummation as written in Eq. (16) (with $R_{F(s)}$ instead of $R_S$ there). Since we know the N$^3$LO TPS of $R_{F(s)}(b)$, we can evaluate this function as TPS, or as Padé [2/1] (the Padé [1/2] is disfavored due to a more complicated and unstable pole structure).

The results for the soft binding energy $E_{b\bar{b}}(s)$ of the ground state of bottonium, as functions of the renormalization scale $\mu$, are presented in Fig. 6(a). The values of input

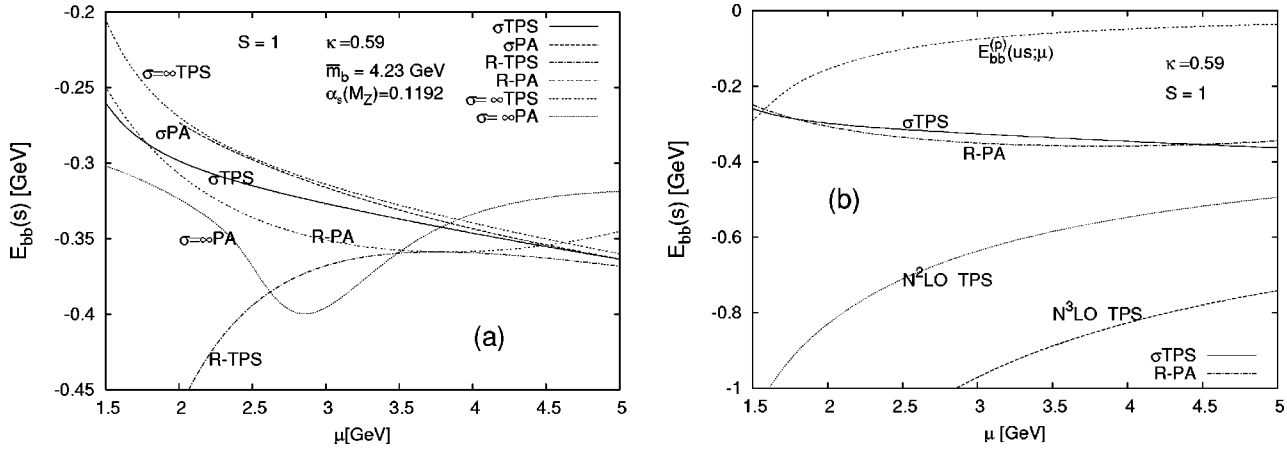


FIG. 6. (a) Soft part $E_{b\bar{b}}(s)$ of the ground state binding energy of $b\bar{b}$, evaluated with four different methods involving (PV) Borel resummation, as functions of the renormalization scale $\mu$. Details are given in the text. In (b) the simple TPS results for $E_{b\bar{b}}(s)$ are included [Eq. (37)], as well as the "perturbative" ultrasoft part $E^{(p)}_{b\bar{b}}(us;\mu)$ [Eq. (38)].

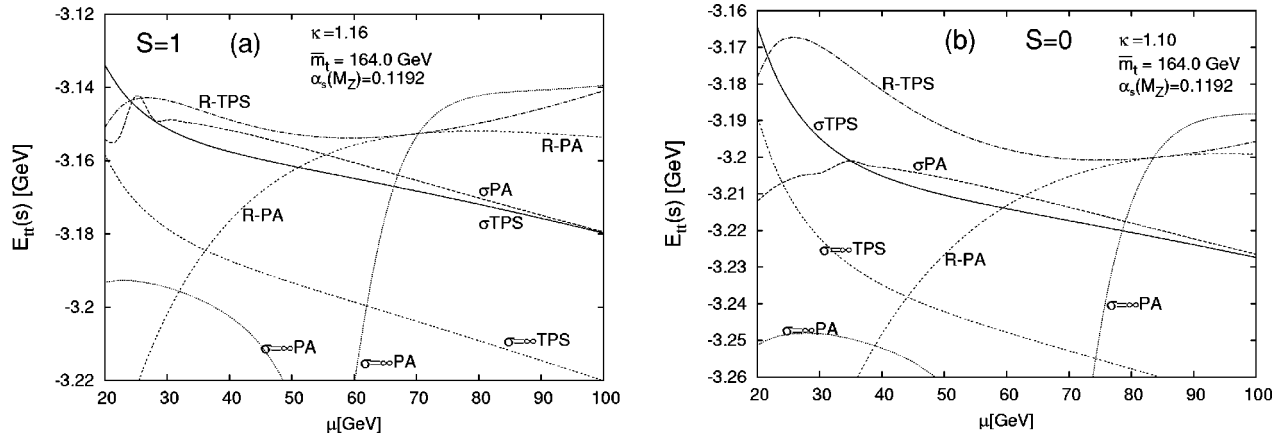


FIG. 7. Same as in Fig. 6(a), but for the toponium system–(a) vector ($S=1$), (b) scalar ($S=0$). Details are given in the text.

parameters are taken as in Figs. 2 and 5(a), and for the "$\sigma$-regularized" method we take $\sigma=0.36$ according to Eq. (36a) (note that the $R$-method does not need $N_m$, $c_4$, and $\sigma$ as input). For each of the three methods, we present two curves: when the analytic part is evaluated as TPS, or as Padé [2/1] (PA), where the role of the analytic part in the $R$-method is taken over by the function $R_{F(s)}(b)$ itself. We observe from the figure that the bilocal method (33) ($\sigma=\infty$) gives the TPS and PA results which significantly differ from each other. On the other hand, the "$\sigma$-regularized" method (35) ($\sigma=0.36$) gives the TPS and PA results closer to each other. The methods $\sigma$-TPS, $\sigma$-PA, and $R$-PA give similar results in the entire presented $\mu$-interval. $R$-TPS appears to fail at low $\mu$ ($\approx m_b\alpha_s\approx 1-2$ GeV). In Fig. 6(b) we include, for comparison, the simple TPS evaluation of $E_{b\bar{b}}(s)$, according to formula [cf. Eq. (26)]

$$F(s)^{(\mathrm{TPS})}\equiv -\frac{9}{4\pi}\frac{1}{\overline{m}_b\alpha_s(\tilde{\mu})}E_{q\bar{q}}(s)=a(\mu)[1+a(\mu)f_1 + a^2(\mu)f_2+a^3(\mu)f_3], \tag{37}$$

where for N$^2$LO TPS case we take $f_3=0$. In Fig. 6(b) the same input parameters are used as in Fig. 6(a). We see that the perturbation series shows strongly divergent behavior already at N$^3$LO. In this figure, we also included the "perturbative" ultrasoft part $E^{(\mathrm{p})}_{b\bar{b}}(us;\mu)$ calculated according to [see Eqs. (24) and (25b)].

$$F^{(\mathrm{p})}(us)\equiv -\frac{9}{4\pi}\frac{1}{\overline{m}_b\alpha_s(\tilde{\mu})}E^{(\mathrm{p})}_{qq}(us;\mu)=k_{3,0}a^4(\mu). \tag{38}$$

This quantity is highly $\mu$-dependent. We return to the discussion of the $us$ energy part in Sec. IV B.

In Figs. 7(a), (b), we present, in analogy with Fig. 6(a), the results for the vector and scalar toponium soft binding energy, respectively. The values of the input parameters are the same as in Figs. 3, 4, and in addition $\sigma=0.33$ according to Eq. (36b). The comparative qualitative behavior of the results of various methods is similar as in the bottonium case, except that now $R$-PA method appears to fail at low renormalization scales $\mu\approx m_t\alpha_s\approx 30$ GeV while $R$-TPS maintains more $\mu$-stability there.

In Fig. 8(a) we present the results analogous to Fig. 7(a) ($S=1$ case), where we now include the results of the simple TPS evaluation (37) for $t\bar{t}$. In Fig. 8(b), we present the result

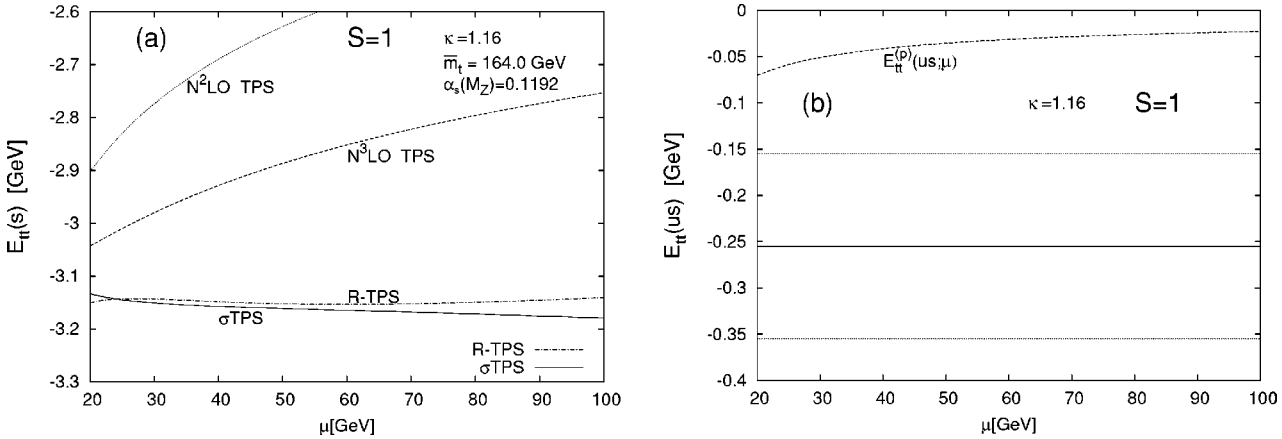


FIG. 8. (a) Same as in Fig. 7(a), but now the results of the simple TPS evaluation (37) are included. (b) The ultrasoft energy parts by different evaluations: $E^{(\mathrm{p})}_{t\bar{t}}(us;\mu)$ by Eq. (38); $E_{t\bar{t}}(us)$ values of Eq. (48a) as straight lines. The input parameters are the same as in Fig. 7(a).

TABLE II. The separate uncertainties $\delta\overline{m}_b$ (in MeV) for the extracted value of $\overline{m}_b$ from various sources: 1) *us* $[E_{b\bar{b}}(us)^{(\mathrm{p+np})} = -100 \pm 106$ MeV]; 2) $\mu = 3 \pm 1$ GeV; (3) $\mu_m = \overline{m}_b(1 \pm 0.5)$; 4) $\alpha_s(m_\tau) = 0.3254 \pm 0.0125$ $[\alpha_s(M_Z) = 0.1192 \pm 0.0015]$; 5) $N_m = 0.555 \pm 0.020$ $[\kappa = 0.59 \pm 0.19]$; 6) $a_3/4^3 = 86 \pm 23$; 7) $c_4 = 40 \pm 60$; 8) $\sigma = 0.36 \pm 0.03$; 9) $m_c \neq 0$ ($\delta M_\Upsilon(m_c \neq 0) = \pm 10$ MeV).

| | *us* | $\mu$ | $\mu_m$ | $\alpha_s$ | $N_m$ | $a_3$ | $c_4$ | $\sigma$ | $m_c$ |
|---|---|---|---|---|---|---|---|---|---|
| $\sigma$-TPS | −49 | +9 | −4 | −13 | −3 | +2 | −8 | +4 | −5 |
| | +49 | −13 | +2 | +14 | +2 | −2 | +8 | −9 | +5 |
| $\sigma$-PA | −49 | +13 | −4 | −15 | −3 | +1 | −5 | +5 | −5 |
| | +49 | −20 | +2 | +15 | +2 | −1 | +2 | −9 | +5 |
| *R*-TPS | −50 | −4 | +4 | −8 | −9 | −3 | 0 | 0 | −5 |
| | +50 | +45 | −40 | +10 | +11 | +3 | 0 | 0 | +5 |
| *R*-PA | −49 | +3 | +4 | −11 | −4 | −2 | 0 | 0 | −5 |
| | +49 | −20 | −40 | +12 | +4 | +2 | 0 | 0 | +5 |

for the ''perturbative'' ultrasoft part $E_{t\bar{t}}^{(\mathrm{p})}(us;\mu)$ calculated according to Eq. (38) for the $t\bar{t}$ system (dashed $\mu$-dependent line). We further include there the more realistic estimates obtained later in Sec. IV C [Eq. (48a)].

### B. Extraction of bottom mass

We need to address now also the problem of evaluating the ultrasoft part $E_{q\bar{q}}(us)$ of the ground state binding energy. The estimate of the perturbative part is given in Eq. (27), where it was essential to take for the renormalization scale a *us* scale $\mu \sim \mu_{us} \sim m_q \alpha_s^2$.

For the bottonium case, this scale is below 1 GeV, the energy at which we cannot determine perturbatively $\alpha_s(\mu)$. This indicates that in the bottonium the *us* part of the binding energy has an appreciable nonperturbative part. The lowest energy at which we can still determine perturbatively $\alpha_s$ is $\mu \approx 1.5$–$2.0$ GeV, giving $\alpha_s(\mu) \approx 0.30 - 0.35$. Although this is a soft scale for $b\bar{b}$, we will use this also as an ultrasoft scale. Then by Eq. (27)

$$E_{b\bar{b}}(us)^{(\mathrm{p})} \approx -\frac{4}{9}\overline{m}_q \pi^2 k_{3,0}(us) a^5(\mu_{us}) \approx (-150 \pm 100)\ \mathrm{MeV}. \quad (39)$$

The nonperturbative contribution coming from the gluonic condensate is given by [53]

$$E_{b\bar{b}}(us)^{(\mathrm{np})} \approx \overline{m}_b \pi^2 \frac{624}{425}\left(\frac{4}{3}\overline{m}_b \alpha_s(\mu_{us})\right)^{-4} \langle a(\mu_{us}) G_{\mu\nu} G^{\mu\nu} \rangle \approx (50 \pm 35)\ \mathrm{MeV}, \quad (40)$$

where we used $\overline{m}_b = 4.2$ GeV, and the value of the gluon condensate $\langle (\alpha_s/\pi) G^2 \rangle = 0.009 \pm 0.007$ GeV$^4$ [54]. Equations (39) and (40) give

$$E_{b\bar{b}}(us)^{(\mathrm{p+np})} \approx (-100 \pm 106)\ \mathrm{MeV}, \quad (41)$$

where the two uncertainties were added in quadrature. In addition, there are finite charm mass contributions which have been calculated in Ref. [55] (based on the results of Refs. [7,56,57]). These contributions modify the values of $m_b$ and $E_{b\bar{b}}$, resulting in the contribution to the mass $M_\Upsilon(1S) = (2m_b + E_{b\bar{b}})$,

$$\delta M_\Upsilon(1S, m_c \neq 0) \approx 25 \pm 10\ \mathrm{MeV}. \quad (42)$$

The estimates (41), and (42) then give a rough estimate of the *us* and $m_c \neq 0$ contributions to the bottonium mass $\delta M_\Upsilon(1S; us + m_c) \approx (-75 \pm 106)$ MeV. The mass of the $\Upsilon(1S)$ vector bottonium ground state is well measured $M_\Upsilon(1S) = 9460$ MeV with virtually no uncertainty [58]. Therefore, the pure perturbative ''soft'' mass is

$$M_\Upsilon(1S; s) = 2m_b + E_{b\bar{b}}(s) = 9535 \mp 106\ \mathrm{MeV}, \quad (43)$$

where the uncertainty $\pm 106$ MeV is the rough estimate dominated by the uncertainty of the *us* regime contribution. Our numerical results for $E_{b\bar{b}}(s)$ in this section and for $m_b$ presented in Sec. II allow us, by varying the input value of $\overline{m}_b$, to adjust the sum $2m_b + E_{b\bar{b}}(s)$ to the value given in Eq. (43). For the soft binding energy we apply the $\sigma$-regularized bilocal methods $\sigma$-TPS and $\sigma$-PA, and *R*-TPS and *R*-PA, with the aforementioned ''central'' input parameters: $\alpha_s(M_Z) = 0.1192$; $\tilde{\mu} = 1.825$ GeV ($\approx \mu_s$), thus $\alpha_s(\tilde{\mu}, n_f = 4) = 0.3263$ $[\alpha_s(\mu_s) = 0.326]$; $N_m = 0.555$; $\kappa = 0.59$; $\sigma = 0.36$; $a_3/4^3 = 86$; $c_4(\overline{\mathrm{MS}}) = 40$. For $2m_b$ we apply the bilocal-TPS and *R*-TPS method, with renormalization scale $\mu_m/\overline{m}_b = 1$, both methods giving us very similar results [cf. Fig. 1 (a)]. The bilocal-TPS method is applied for $2m_b$ when $\sigma$-TPS and $\sigma$-PA are applied for $E_{b\bar{b}}(s)$; the *R*-TPS is applied for $2m_b$ when *R*-TPS and *R*-PA are applied for $E_{b\bar{b}}(s)$ (the same combinations of methods will be applied in the Sec. IV C to the study of toponium). The extracted values of $\overline{m}_b \equiv \overline{m}_b(\mu = \overline{m}_b)$ are then

$$\overline{m}_b = 4.225 \pm 0.054\ \mathrm{GeV}\quad (\sigma\text{-TPS}) \quad (44a)$$

$$= 4.220 \pm 0.056\ \mathrm{GeV}\quad (\sigma\text{-PA}) \quad (44b)$$

$$= 4.243 \pm 0.080\ \mathrm{GeV}\quad (R\text{-TPS}) \quad (44c)$$

$$= 4.235 \pm 0.068\ \mathrm{GeV}\quad (R\text{-PA}). \quad (44d)$$

TABLE III. The uncertainty $\delta E_{t\bar{t}}(us)$ and the separate uncertainties in $\delta E_{t\bar{t}}(s)$ (in MeV) for the toponium $S=1$ binding energy from various sources: 1) $\delta E_{t\bar{t}}(us)$ [cf. Eqs. (48)]; 2) $\mu=55\pm20$ GeV; 3) $\alpha_s(M_Z)=0.1192\pm0.0015$; 4) $N_m=0.533\pm0.020$ [$\kappa=1.16^{+0.31}_{-0.29}$]; 5) $a_3/4^3=62.5\pm20$; 6) $c_4=70\pm20$; 7) $\sigma=0.33\pm0.03$. The pole mass $m_t$ is kept fixed at the value $m_t=174.30$ GeV.

| | | $\delta E(s)$ | | | | | |
|---|---|---|---|---|---|---|---|
| | $\delta E(us)$ | $\mu$ | $\alpha_s$ | $N_m$ | $a_3$ | $c_4$ | $\sigma$ |
| $\sigma$-TPS | −100 | −7 | −105 | −21 | −4 | +5 | −17 |
| | +100 | +8 | +109 | +23 | +4 | −5 | +29 |
| $\sigma$-PA | −100 | −10 | −105 | −21 | −3 | +3 | −16 |
| | +100 | +8 | +109 | +22 | +3 | −2 | +26 |
| $R$-TPS | −100 | +3 | −104 | −21 | −8 | 0 | 0 |
| | +100 | +8 | +109 | +26 | +8 | 0 | 0 |
| $R$-PA | −100 | +7 | −105 | −18 | −6 | 0 | 0 |
| | +100 | −28 | +110 | +20 | +7 | 0 | 0 |

The uncertainties are the combination, in quadrature, of uncertainties from various sources, shown in Table II for each of the four methods. In the case of asymmetric uncertainties, the larger is taken. The largest uncertainty ($\pm0.049$ GeV) comes from the *us* sector uncertainty $\pm0.106$ GeV of Eq. (41). In the case of *R*-TPS method, the variation of the soft binding energy with the variation of the renormalization scale is a competing source of uncertainty for $\overline{m}_b$ ($\pm0.045$ GeV), and in the case of *R*-TPS and *R*-PA methods (where $m_t$ is resummed by *R*-TPS) the uncertainty from the variation of the renormalization scale $\mu_m$ in the $2m_t$-resummation is competing as well (0.040 GeV). The arithmetic average of the central values of Eq. (44) gives us

$$\overline{m}_b=4.231\pm0.068\ \text{GeV}\quad(\text{our average}),\tag{45}$$

where we emphasize that the central value for the strong coupling parameter was chosen to be $\alpha_s(M_Z)=0.1192$. In Eq. (45), the uncertainty was chosen to be the second largest uncertainty in Eq. (44). The largest uncertainty, $\pm0.080$ GeV of the *R*-TPS method, was discarded because *R*-TPS is the only one of the four methods which fails simultaneously at the low $\mu_m$ ($<\overline{m}_b$) and low $\mu$ ($<3$ GeV) renormalization scales.

### C. Numerical results for the toponium

For the binding energy of the toponium, the numerical results are obtained in the following way. First the value of the (PV) pole mass $m_t$ is fixed to the central experimental value $m_t=174.3$ GeV [58]. For calculation of the binding energy, $\overline{m}_t$ is an input parameter (but not $m_t$). When $\alpha_s$ varies [$\alpha_s(M_Z)=0.1192\pm0.0015$], the two methods of Sec. II [cf. Fig. 1(b)], with the renormalization scale $\mu_m=\overline{m}_t$, give $\overline{m}_t=164.000^{-0.153}_{+0.163}$ GeV (bilocal method) and $\overline{m}_t=164.011^{-0.153}_{+0.162}$ GeV (*R*-method), when $m_t=174.3$ GeV (PV value). The values of $\overline{m}_t$ change by 0.020 GeV or less when the other parameters are varied (renormalization scale $\mu_m$; $N_m$ and $c_4$ for bilocal method; see Sec. II), and such small variation in $\overline{m}_t$ influences the toponium binding energy insignificantly[5]–by less than 0.001 GeV.

We use as the central $\overline{m}_t$ input value $\overline{m}_t=164.000$ GeV to calculate $E_{t\bar{t}}(s)$ with the four aforementioned Borel methods, using for other input parameters their "central" values used in Figs. 5(b), 7: $\alpha_s(M_Z)=0.1192$; $\tilde{\mu}=31$ GeV ($\approx\mu_s$), thus $\alpha_s(\tilde{\mu},n_f=5)=0.143$ [$\alpha_s(\mu_s)=0.14$]; $N_m=0.533$; $\kappa=1.16$ ($S=1$),1.10 ($S=0$); $\mu=55$ GeV ($S=1$), 65 GeV ($S=0$); $\sigma=0.33$; $a_3/4^3=62.5$; $c_4(\overline{\text{MS}})=70$. Then the resulting toponium soft energy is

$$E_{t\bar{t}}(s)=-3.163\pm0.116\ \text{GeV}\ (-3.216\pm0.120\ \text{GeV})\quad(\sigma\text{-TPS})\tag{46a}$$

$$=-3.158\pm0.115\ \text{GeV}\ (-3.212\pm0.118\ \text{GeV})\quad(\sigma\text{-PA})\tag{46b}$$

$$=-3.154\pm0.113\ \text{GeV}\ (-3.200\pm0.116\ \text{GeV})\quad(R\text{-TPS})\tag{46c}$$

$$=-3.159\pm0.115\ \text{GeV}\ (-3.209\pm0.118\ \text{GeV})\quad(R\text{-PA}),\tag{46d}$$

where the results are given for the vector ($S=1$) case and in parentheses for the scalar ($S=0$) toponium case. The uncertainties are combinations, in quadrature, of uncertainties coming from various input sources: $\delta\alpha_s$, $\delta\mu$, $\delta a_3$, $\delta c_4$, $\delta N_m$, and $\delta\sigma$. When $\delta\alpha_s$ is varied, the value $\overline{m}_t$ is varied as well, as described above, but otherwise it is kept fixed (at 164.000 GeV). All the corresponding separate uncertainties $\delta E_{t\bar{t}}(s)$ are given in Tables III for $S=1$ and IV for $S=0$. The ultrasoft part $E_{t\bar{t}}(us)$ is principally perturbative and can be estimated by formula (27) where the *us* coefficient is

[5]A variation $\delta\overline{m}_t\pm10.0$ MeV results in $\delta E_{t\bar{t}}(s)=\mp0.11$ MeV, when all other input parameters are kept fixed.

TABLE IV. As Table III, but for $S=0$. The input parameters are the same, except for $\mu$ ($=65 \pm 20$ GeV) and $\kappa$ ($=1.10^{+0.39}_{-0.33}$, corresponding to $N_m=0.533\pm0.020$).

| | | $\delta E(s)$ | | | | | |
|---|---|---|---|---|---|---|---|
| | $\delta E(us)$ | $\mu$ | $\alpha_s$ | $N_m$ | $a_3$ | $c_4$ | $\sigma$ |
| $\sigma$-TPS | $-110$ | $-6$ | $-107$ | $-23$ | $-3$ | $+5$ | $-17$ |
| | $+110$ | $+8$ | $+112$ | $+26$ | $+4$ | $-5$ | $+31$ |
| $\sigma$-PA | $-110$ | $-8$ | $-107$ | $-23$ | $-2$ | $+4$ | $-16$ |
| | $+110$ | $+8$ | $+112$ | $+25$ | $+3$ | $-2$ | $+28$ |
| $R$-TPS | $-110$ | 0 | $-106$ | $-25$ | $-7$ | 0 | 0 |
| | $+110$ | $+13$ | $+111$ | $+30$ | $+8$ | 0 | 0 |
| $R$-PA | $-110$ | $+9$ | $-107$ | $-20$ | $-6$ | 0 | 0 |
| | $+110$ | $-27$ | $+112$ | $+23$ | $+6$ | 0 | 0 |

given by (24). This part is more manageable than in the bottonium case, because the typical *us* energy now is still in the perturbative regime: $\mu_{us}\sim 10^1$ GeV. We determine this energy by the condition

$$\mu_{us}=\kappa' \overline{m}_t \alpha_s^2(\mu_{us}), \tag{47}$$

where $\kappa'\sim 1$. The value $\kappa'=1$ corresponds to $\mu_{us}\approx 7$ GeV. Equations (27) and (24) then give for the value $E_{t\bar{t}}(us)=-0.255$ GeV ($S=1$) and $-0.272$ GeV ($S=0$). When we change to $\kappa'=2$ ($\mu_{us}=10.5$ GeV), the values of $E_{t\bar{t}}(us)$ go up by 0.100 and 0.110 for the $S=1,2$, respectively. This we adopt as the uncertainty in the *us* sector. Therefore, we have by Eq. (27)

$$E_{t\bar{t}}(us)=-0.255\pm 0.100 \text{ GeV} \quad (S=1) \tag{48a}$$

$$=-0.272\pm 0.110 \text{ GeV} \quad (S=0), \tag{48b}$$

corresponding to $\mu_{us}=7.0^{+3.5}_{-1.5}$ GeV. When we take for the soft part $E_{t\bar{t}}(s)$ the arithmetic average of the results of the four methods (46), and combining it with the ultrasoft part (48), we obtain

$$E_{t\bar{t}}=-3.413\pm 0.153 \text{ GeV} \quad (S=1) \tag{49a}$$

$$=-3.481\pm 0.163 \text{ GeV} \quad (S=0). \tag{49b}$$

The two dominant contributions to the uncertainties in Eq. (49) are the uncertainty from $\alpha_s$ in the soft sector, and the uncertainty of the ultrasoft sector, as seen from Tables III and IV and Eq. (48).

The results (49) are relevant for the future determinations of $\overline{m}_t$ from $t\bar{t}$ production near threshold. We recall that the determination of the pole mass $m_t$ has, due to the $b=1/2$ renormalon singularity, an intrinsic ambiguity of order $\Lambda_{\rm QCD}$, i.e., several hundred MeV, and cannot be determined from experiments with a higher accuracy. But the mass $\overline{m}_t$ could be eventually determined with accuracy of less than 100 MeV, as pointed out in Ref. [46] where toponium mass was investigated using large-$\beta_0$ arguments. The $S=1$ toponium state is produced in $e^+e^-$ annihilation, while the $S=0$ state in unpolarized $\gamma\gamma$ collisions. The produced resonance is not exactly at the ground state mass value $(2m_t+E_{t\bar{t}})$ because of the large decay width of the toponium [59,60]

$$E_{\rm res.}=2m_t+E_{t\bar{t}}+\delta^\Gamma E_{\rm res.}. \tag{50}$$

The shift in Eq. (50) is $\delta^\Gamma E_{\rm res.}=100\pm 10$ MeV [35,61] and it is rather stable under the variation of all input parameters, including $\alpha_s$ and $\overline{m}_t$. At this point, we should evaluate the sum $(2m_t+E_{t\bar{t}})$ for a general input value of $\overline{m}_t$ ($\approx 164$ GeV). The expected central values of $(2m_t+E_{t\bar{t}})$ can be inferred from the central values of the binding energies (49) which were obtained with the choice $\overline{m}_t=164.000$ GeV. We obtain the variation

$$\delta(2m_t+E_{t\bar{t}})\approx \pm 2.09\,\delta\overline{m}_t, \tag{51}$$

when only the input parameter $\overline{m}_t$ is varied around its central value 164.00 GeV, while all the other input parameters ($\alpha_s$, $N_m$, $\mu_m$, $\mu$, $a_3$, $c_4$, $\sigma$) are kept fixed at their corresponding central values.[6] At $\overline{m}_t=164.000$ GeV, the bilocal method gives $m_t=174.300$ GeV and the $R$-method $m_t=174.288$ GeV. Thus, combining the average of this with relations (51) and (49), we expect the approximate central values $(2m_t+E_{t\bar{t}})=345.175$ GeV for $S=1$ and 345.107 GeV for $S=0$, when $\overline{m}_t=164.000$ GeV. The uncertainties of $(2m_t+E_{t\bar{t}})$ originate from the variation of all the input parameters except $\overline{m}_t$. Some of them are expected to be close to the uncertainties in Eq. (49) given for the binding energies. However, they are not equal to these uncertainties of Eq. (49) because the latter were obtained by keeping the pole mass fixed ($m_t=174.3$ GeV). Now, however, $\overline{m}_t=164.0$ GeV is kept fixed, and variations of $E_{t\bar{t}}$ and $m_t$ become correlated in the sum $(2m_t+E_{t\bar{t}})$. More importantly, the variation of $\alpha_s$ now changes $E_{t\bar{t}}(s)$ and $2m_t$, and, to a lesser degree, $E_{t\bar{t}}(us)$; the variation of $N_m$ changes $\kappa$ which

[6]More precisely, $\delta\overline{m}_t=\pm 100$ MeV would correspond to $\delta(2m_t+E_{t\bar{t}})\approx\pm 208.8$ MeV, of which $\delta(2m_t)=\pm 210.1$ MeV, $\delta E_{t\bar{t}}(s)=\mp 1.1$ MeV, and $\delta E_{t\bar{t}}(us)=\mp 0.2$ MeV.

TABLE V. The separate uncertainties $\delta[2m_t+E_{t\bar{t}}(s+us)]$ (in MeV) for the toponium $S=1$ mass from various sources: 1) $\mu_{us}=7.0^{-1.5}_{+3.5}$ GeV [cf. Eq. (48)]; 2) $\mu=55\pm20$ GeV; 3) $\mu_m=\overline{m}_b(1\pm0.5)$; 4) $\alpha_s(M_Z)=0.1192\pm0.0015$; 5) $N_m=0.533\pm0.020$ [$\kappa=1.16^{+0.31}_{-0.29}$]; 6) $a_3/4^3=62.5\pm20$; 7) $c_4=70\pm20$; 8) $\sigma=0.33\pm0.03$. The input mass $\overline{m}_t=164.00$ GeV is kept fixed.

| | $\mu_{us}$ | $\mu$ | $\mu_m$ | $\alpha_s$ | $N_m$ | $a_3$ | $c_4$ | $\sigma$ |
|---|---|---|---|---|---|---|---|---|
| $\sigma$-TPS | −100 | −7 | +13 | +188 | +94 | −4 | +3 | −17 |
| | +100 | +8 | −9 | −203 | −108 | +4 | −3 | +30 |
| $\sigma$-PA | −100 | −10 | +13 | +189 | +94 | −3 | +1 | −16 |
| | +100 | +8 | −9 | −203 | −108 | +3 | −1 | +26 |
| $R$-TPS | −100 | +2 | −9 | +188 | +54 | −8 | 0 | 0 |
| | +100 | +7 | −95 | −203 | −65 | +8 | 0 | 0 |
| $R$-PA | −100 | +6 | −9 | +187 | +57 | −7 | 0 | 0 |
| | +100 | −29 | −95 | −202 | −71 | +6 | 0 | 0 |

in turn changes $E_{t\bar{t}}(us)$ [Eqs. (27) and (24)] and, to a lesser degree, $E_{t\bar{t}}(s)$ and $2m_t$. The explicit calculations give for $S=1$,

$$(2m_t+E_{t\bar{t}})=345.181\pm0.253\ \text{GeV}\quad(\sigma\text{-TPS}) \tag{52a}$$

$$=345.186\pm0.253\ \text{GeV}\quad(\sigma\text{-PA}) \tag{52b}$$

$$=345.168\pm0.254\ \text{GeV}\quad(R\text{-TPS}) \tag{52c}$$

$$=345.163\pm0.256\ \text{GeV}\quad(R\text{-PA}), \tag{52d}$$

and for $S=0$,

$$(2m_t+E_{t\bar{t}})=345.119\pm0.263\ \text{GeV}\quad(\sigma\text{-TPS}) \tag{53a}$$

$$=345.116\pm0.263\ \text{GeV}\quad(\sigma\text{-PA}) \tag{53b}$$

$$=345.105\pm0.261\ \text{GeV}\quad(R\text{-TPS}) \tag{53c}$$

$$=345.096\pm0.263\ \text{GeV}\quad(R\text{-PA}). \tag{53d}$$

Here, the resummation of the mass $2m_t$ was performed by the bilocal TPS method in the first two cases [Eqs. (52a), (52b) and (53a), (53b)], and by the $R$-TPS method in the last two cases [Eqs. (52c), (52d) and (53c), (53d)]—cf. Sec. II. In Tables V and VI we give, for $S=1$ and $S=0$, respectively, separate uncertainties in the mass $(2m_t+E_{t\bar{t}})$ coming from the corresponding variations of the input parameters $\alpha_s$, $N_m$, $\mu_m$, $\mu$, $a_3$, $c_4$, $\sigma$ and $\mu_{us}$. Adding them in quadrature, this gave the uncertainties in Eqs. (52a)–(53d). We take the arithmetic average of the central values in Eqs. (52a)–(52d) for $S=1$, and of the central values in Eqs. (53a)–(53d) for $S=0$,

$$(2m_t+E_{t\bar{t}})=345.175\pm0.256\ \text{GeV}\quad(S=1), \tag{54a}$$

$$(2m_t+E_{t\bar{t}})=345.109\pm0.263\ \text{GeV}\quad(S=0). \tag{54b}$$

Combining this with Eq. (51) and the aforementioned shift value $\delta^{\Gamma}E_{\text{res.}}=100\pm10$ MeV in Eq. (50), this gives finally

$$E_{\text{res.}}=(345.28\pm0.26)\ \text{GeV}+2.09(\overline{m}_t-164.00\ \text{GeV})\times(S=1) \tag{55a}$$

$$=(345.21\pm0.26)\ \text{GeV}+2.09(\overline{m}_t-164.00\ \text{GeV})\times(S=0), \tag{55b}$$

In Tables V and VI we see that the major source of uncertainty is from the uncertainty $\delta\alpha_s(M_Z)=\pm0.0015$, followed by the uncertainty of the ultrasoft sector scale $\delta\mu_{us}$ [cf. Eq. (48)] and in the $\sigma$-methods by the uncertainty in the renormalon residue parameter $\delta N_m=\pm0.020$ and in $R$-methods by the uncertainty $\delta\mu_m$ in the renormalization scale for the resummation of $2m_t$.

TABLE VI. As Table V, but for $S=0$. The input parameters are the same, except for $\mu$ ($=65\pm20$ GeV) and $\kappa$ ($=1.10^{+0.39}_{-0.33}$, corresponding to $N_m=0.533\pm0.020$).

| | $us$ | $\mu$ | $\mu_m$ | $\alpha_s$ | $N_m$ | $a_3$ | $c_4$ | $\sigma$ |
|---|---|---|---|---|---|---|---|---|
| $\sigma$-TPS | −110 | −7 | +13 | +184 | +112 | −4 | +3 | −18 |
| | +110 | +7 | −9 | −199 | −127 | +3 | −4 | +30 |
| $\sigma$-PA | −110 | −9 | +13 | +184 | +112 | −3 | +1 | −17 |
| | +110 | +7 | −9 | −199 | −128 | +2 | −1 | +27 |
| $R$-TPS | −110 | 0 | −8 | +184 | +71 | −7 | 0 | 0 |
| | +110 | +13 | −95 | −199 | −83 | +8 | 0 | 0 |
| $R$-PA | −110 | +9 | −9 | +183 | +75 | −6 | 0 | 0 |
| | +110 | −27 | −95 | −198 | −90 | +6 | 0 | 0 |

TABLE VII. Recently obtained values of ($\overline{\text{MS}}$) $\overline{m}_b$ mass obtained from $\Upsilon$ sum rules or from spectrum of the $\Upsilon(1S)$ resonance. Wherever needed ( [14,35]), the central mass values were adjusted to the common input central value $\alpha_s(M_Z)=0.118$.

| Reference | Method | Order | $\overline{m}_b(\overline{m}_b)$ (GeV) |
|---|---|---|---|
| PP98 [43] | $\Upsilon$ sum rules | NNLO | $4.21\pm0.11$ |
| MY98 [42] | $\Upsilon$ sum rules | NNLO | $4.20\pm0.10$ |
| BS99 [67] | $\Upsilon$ sum rules | NNLO | $4.25\pm0.08$ |
| H00 [57] | $\Upsilon$ sum rules | NNLO | $4.17\pm0.05$ |
| KS01 [68] | $\Upsilon$ sum rules | NNLO | $4.209\pm0.050$ |
| CH02 [69] | $\Upsilon$ sum rules | NNLO | $4.20\pm0.09$ |
| E02 [70] | $\Upsilon$ sum rules | NNLO | $4.24\pm0.10$ |
| P01 [13] | spectrum, $\Upsilon(1S)$ | NNLO | $4.210\pm0.090\pm0.025$ |
| BSV01 [55] | spectrum, $\Upsilon(1S)$ | NNLO | $4.190\pm0.020\pm0.025$ |
| PS02 [35] | spectrum, $\Upsilon(1S)$ | $\text{N}^3\text{LO}$ | $4.349\pm0.070$ |
| L03 [14] | spectrum, $\Upsilon(1S)$ | $\text{N}^3\text{LO}$ | $4.19\pm0.04$ |
| This work, Eq. (56) | spectrum, $\Upsilon(1S)$ | $\text{N}^3\text{LO}$ | $4.241\pm0.070$ |

We could adopt in the ultrasoft regime a more conservative approach, allowing for the parameter $\kappa'$ in Eq. (47) not just to vary from value 1 up to value 2, but also to vary down to value 1/2. This would correspond to the variation of $\mu_{us}$ from 7 GeV down to 4.27 GeV [thus increasing $\alpha_s(\mu_{us})$ from 0.198 to 0.228, if keeping $n_f=5$]. This would increase the uncertainties $\pm0.100$ and $\pm0.110$ GeV in Eq. (48) to $\pm0.260$ and $\pm0.275$ GeV, respectively. This would give in our results (55) for the $t\bar{t}$ resonance the increased uncertainties 0.35 GeV ($S=1$) and $\pm0.36$ GeV ($S=0$).

The present experimental uncertainty in the pole mass is $\delta m_t=5.1$ GeV [58], corresponding to $\delta\overline{m}_t=4.86$ GeV (provided we consider $m_t$ to be the principal value pole mass). This implies, according to results (55), the present experimental uncertainty $(\delta E_{\text{res.}})_{\text{exp.}}=\pm10.16$ GeV, which is still very much above the uncertainties $\pm0.26$ GeV (or $\pm0.36$ when conservative approach in the *us* regime) coming from the uncertainties of the resummation methods and of the input parameters (other than $\overline{m}_t$).

In this work we did not include electroweak (Higgs) effects, which are significant in the case of the top quark. In Refs. [62,63] the $\mathcal{O}(\alpha)$ and $\mathcal{O}(\alpha\alpha_s)$ corrections, respectively, to the relation between $m_t$ and $\overline{m}_t$ mass were calculated. The size of these corrections significantly depends on the hitherto unknown mass $M_H$. For low Higgs masses $M_H=100$–$300$ GeV, these corrections change the value of $m_t$, for a given value of $\overline{m}_t$, by several percent. Inclusion of these effects would be important for a realistic extraction of $\overline{m}_t$ from the resonance energy of the $t\bar{t}$ production.[7]

## V. COMPARISONS AND CONCLUSIONS

In this section we will compare our results with some of the results recently published in the literature.

Our results for the mass $\overline{m}_b$, Eqs. (44), (45), Table II, will be compared with those recently obtained by authors who either used pQCD expansions for the $\Upsilon(1\,S)$ resonance mass, or $\Upsilon$ sum rules. The only input parameter common to all these methods is $\alpha_s$. The comparison of the various methods is more reasonable if the same central input value of ($\overline{\text{MS}}$) $\alpha_s(M_Z)$ is taken. Our central value was $\alpha_s(m_\tau)=0.3254$ [$\Rightarrow\alpha_s(M_Z)=0.1192$] since such [34], or similar [20,64], values follow from the (nonstrange) semihadronic $\tau$ decay data which are very precise [65]. On the other hand, the world average as of September 2002 is $\alpha_s(M_Z)=0.1183\pm0.0027$ [66]. Most of the authors during the last four years used central value $\alpha_s(M_Z)\approx0.118$. Therefore, for comparisons, we convert our results (44) to this central value of $\alpha_s$–more specifically, from $\alpha_s(M_Z)=0.1192\pm0.0015$ to $0.1180\pm0.0015$. This can be easily done by inspecting in Table II the column under $\alpha_s$, giving in Eqs. (44a)–(44d) an increase in the central values of 11, 12, 8 and 10 MeV, respectively. This gives the average 10 MeV higher than in Eq. (45)

$$\overline{m}_b=4.241\pm0.068\ \text{GeV}\quad[\text{average when: }\ \alpha_s(M_Z)=0.1180\pm0.0015]. \tag{56}$$

All the separate uncertainties given in Table II remain, of course, valid also in this translated result. In Table VII, we give comparison of this result with others in the recent literature. All these results have the central value $\alpha_s(M_Z)=0.118$. Wherever the central value of $\alpha_s$ was different [14,35], we performed the corresponding translation. There are two important numerical effects in our result. The first is the separate evaluation of the ''perturbative'' ultrasoft energy part at the corresponding low renormalization energy ($\lesssim2$ GeV), Eqs. (27) and (39). If we had not separated the (''perturbative'') ultrasoft from the soft part of the binding energy, the use of the common renormalization energy scale $\mu$ ($\approx3$ GeV) in the resummation then would have given us the central value of $E_{t\bar{t}}(us)$ by about $+100$ MeV higher. Then the extracted value of $\overline{m}_b$ would have gone down by about 46 MeV, giving the value $\overline{m}_b\approx4.195\pm0.068$, with the

[7]We thank M. Kalmykov for clarifications on this point.

TABLE VIII. Comparison of some of the toponium binding energy values $E_{t\bar{t}}$ recently obtained in the literature. The first two values were correspondingly rescaled to our central input $\alpha_s$-value $\alpha_s(M_Z)=0.1192$, and $m_t=174.3$ GeV.

| Reference | Order | $E_{t\bar{t}}$(GeV) |
|---|---|---|
| PS02 [35] | N$^3$LO | $-3.065\pm0.157$ ($S=1,0$) |
| L03 [14] | N$^3$LO | $-3.21\pm0.15$ ($S=1$) |
| This work, Eq. (49a) | N$^3$LO | $-3.413\pm0.153$ ($S=1$) |
| This work, Eq. (49b) | N$^3$LO | $-3.481\pm0.163$ ($S=0$) |

central value close to that of L03 in Table VII. On the other hand, that latter value is quite clearly lower than the value PS02 in Table VII, by about 150 MeV, principally because of the $b=1/2$ renormalon effect which was taken into account here and in Ref. [14]. Thus, the renormalon effect brings down the extracted central value of $\overline{m}_b$ by about 150 MeV, but the separate evaluation/estimate of the ultrasoft contribution brings it up by about 50 MeV. The renormalon effect can also be understood from Fig. 6(b), which suggests that (at $\mu\approx3$ GeV) the renormalon effect pushes upward the soft binding energy $E_{b\bar{b}}(s)$ by about 300 MeV. We note that PS02 used pole mass $m_b$ in their N$^3$LO TPS evaluation of the mass of the $\Upsilon(1S)$ resonance before extracting the value of $\overline{m}_b$.

Our results for the toponium binding energies are given in Eqs. (46), (48) and (49), in connection with Tables III and IV. The result of Ref. [14] was $E_{t\bar{t}}\approx-3.08\pm0.02$ GeV (for $S=1$), but the central value of $\alpha_s$ used there was $\alpha_s(M_Z)=0.1172$. The result of Ref. [35] was $E_{t\bar{t}}\approx-3.01$ GeV, using the central value $\alpha_s(M_Z)=0.1185$. In Table VIII we present our result (49) together with the results of these two references, in both cases rescaled to the common central $\alpha_s$ value $\alpha_s(M_Z)=0.1192$. We see that in our case the toponium binding energies are significantly lower. This lowering is a combination of the renormalon $b=1/2$ effect and of the ultrasoft effect. Figure 8(a) suggests that the renormalon effect, in comparison to N$^3$LO TPS, brings down the soft binding energy $E_{t\bar{t}}(s)$ by about 150 MeV ($\mu=30$ GeV) and 300 MeV ($\mu=60$ GeV). Further, the ultrasoft effect (48) brought down the binding energy by about 200 MeV. More specifically, when making our resummation with no separation of *s* and *us* parts, and using the common renormalization scale $\mu=50$–$60$ GeV, would give results for the binding energy $E_{t\bar{t}}$ higher by about 200 MeV. The deviation of our result for $E_{t\bar{t}}$ from the result of L03 in Table VIII can be explained principally with the ultrasoft effect, and the deviation from PS02 with combination of both the ultrasoft and the renormalon effect. We note that P02 used in their calculation of $E_{t\bar{t}}$ the N$^3$LO TPS with $\mu\approx30$ GeV and the pole mass $m_t$.

This lower binding energy $E_{t\bar{t}}$ is then reflected in the value of the peak (resonance) position $E_{\text{res.}}$—Eq. (55) and Tables V and VI. For example, Ref. [35] obtains for $m_t=174.3$ GeV [and central value $\alpha_s(M_Z)=0.1192$] the values $E_{\text{res.}}=345.63\pm0.16$ GeV for $S=1$ and 0, while we get the values $345.28\pm0.26$ GeV ($S=1$) and $345.21\pm0.26$ GeV ($S=0$), i.e., lower by 350 and 420 MeV than [35]. In Ref. [60], NNLO results for $E_{\text{res.}}$ of several groups [61,71–74] were compared who used in their calculations various renormalon-free masses for the top quark. Their results were taken for the central input values $\alpha_s(M_Z)=0.1190$ and $\overline{m}_t=165.00$ GeV, and are all around $E_{\text{res.}}\approx345.5$ GeV, with variations, due to the renormalization scale ambiguity, being usually below 10 MeV. For these central input values of $\alpha_s$ and $\overline{m}_t$, our results (55)) (see also Tables V and VI) get modified to $347.34\pm0.26$ GeV ($S=1$) and $347.27\pm0.26$ GeV ($S=0$), i.e., lower by about 200–300 MeV.


## ACKNOWLEDGMENT

We express gratitude to the following persons for helpful communications: M. Beneke, V.M. Braun, M. Neubert, A.A. Penin, A. Pineda, and Y. Sumino. This work was supported in part by FONDECYT (Chile) Grant No. 1010094 (G.C.), project USM No. 110321 of the UTFSM (C.C. and G.C), and Mecesup FSM 9901; P.G. would like to acknowledge the support of I. Schmidt.


## APPENDIX: COEFFICIENTS FOR THE EXPANSION OF THE SOFT BINDING ENERGY

We write down here the explicit coefficients $f_j$ of the expansion (26) for the soft part of the ground state binding energy. The logarithms appearing in these expressions involve three scales [$\mu,\tilde{\mu},\overline{m}_q$ and $\overline{\mu}(\tilde{\mu})=(4/3)\overline{m}_q\alpha_s(\tilde{\mu})$],

$$L_1=\ln\left(\frac{\overline{m}_q}{\overline{\mu}(\tilde{\mu})}\right),\quad L_2=\ln\left(\frac{\overline{m}_q}{\tilde{\mu}}\right),\quad L_\mu=\ln\left(\frac{\overline{m}_q}{\mu}\right). \tag{A1}$$

The coefficients $f_j$ are

$$f_1=\frac{1}{2}(35+22L_1-11L_\mu-11L_2)+\frac{1}{9}(-11-6L_1+3L_\mu+3L_2)n_f, \tag{A2}$$

$$f_2=f_2^{(0)}+f_2^{(1)}n_f+f_2^{(2)}n_f^2, \tag{A3a}$$

$$f_2^{(0)}=[381.674+90.75L_1^2+30.25L_\mu^2+L_1(246.417-121L_\mu-60.5L_2)-48.5L_2+L_\mu(-205.25+60.5L_2)-11.6973S(S+1)], \tag{A3b}$$

$$f_2^{(1)}=[-42.7469-11L_1^2-3.66667L_\mu^2+L_\mu(26.6944-7.33333L_2)+6.80556L_2+L_1(-33.0556+14.6667L_\mu+7.33333L_2)], \tag{A3c}$$

$$f_2^{(2)}=[1.16286+(3/9)L_1^2+(1/9)L_\mu^2+L_1(1-(4/9)L_\mu-(2/9)L_2)+L_\mu(-0.814815+(2/9)L_2)-0.185185L_2]. \tag{A3d}$$

$$f_3 = f_3^{(0)} + f_3^{(1)} n_f + f_3^{(2)} n_f^2 + f_3^{(3)} n_f^3, \tag{A4a}$$

$$\begin{aligned} f_3^{(0)} = [&6726.11 + 665.5 L_1^3 - 166.375 L_\mu (40.8024 \\ &+ (-10.5992 + L_\mu) L_\mu) + L_1^2 (2381.5 \\ &- 1497.38 L_\mu - 499.125 L_2) - 871.429 L_2 \\ &- 499.125 (-1.8843 + L_\mu) L_\mu L_2 \\ &- 201.438 L_2^2 + L_1 (7457.17 - 497.292 L_2 \\ &+ L_\mu (-4346.38 + 998.25 L_\mu + 998.25 L_2)) \\ &- 257.341 (0.211191 + L_1 - 0.75 L_\mu \\ &- 0.25 L_2) S(S+1) - 61.4109 (-6.13937 \\ &+ S(S+1)) \ln(\alpha_s(\mu_s)) + 440.172 \ln(\kappa) \\ &+ 2 a_3 / 4^3], \end{aligned} \tag{A4b}$$

$$\begin{aligned} f_3^{(1)} = [&-1274.33 - 1277.92 L_1 - 471.125 L_1^2 \\ &- 121 L_1^3 + 1182.32 L_\mu + 843.667 L_1 L_\mu \\ &+ 272.25 L_1^2 L_\mu - 335.813 L_\mu^2 - 181.5 L_1 L_\mu^2 \\ &+ 30.25 L_\mu^3 + 124.501 L_2 + 108.361 L_1 L_2 \\ &+ 90.75 L_1^2 L_2 - 186.708 L_\mu L_2 \\ &- 181.5 L_1 L_\mu L_2 + 90.75 L_\mu^2 L_2 + 36.7292 L_2^2 \\ &+ (4.06858 + 15.5964 L_1 - 11.6973 L_\mu \\ &- 3.8991 L_2) S(S+1)], \end{aligned} \tag{A4c}$$

$$\begin{aligned} f_3^{(2)} = [&70.8992 + 70.2453 L_1 + 28.9722 L_1^2 \\ &+ 7.33333 L_1^3 - 65.9925 L_\mu - 51.6667 L_1 L_\mu \\ &- 16.5 L_1^2 L_\mu + 20.5972 L_\mu^2 + 11 L_1 L_\mu^2 \\ &- 1.83333 L_\mu^3 - 5.19388 L_2 - 6.57407 L_1 L_2 \\ &- 5.5 L_1^2 L_2 + 10.9167 L_\mu L_2 + 11 L_1 L_\mu L_2 \\ &- 5.5 L_\mu^2 L_2 - 2.09722 L_2^2], \end{aligned} \tag{A4d}$$

$$\begin{aligned} f_3^{(3)} = [&-1.21475 - 1.21714 L_1 - (5/9) L_1^2 \\ &- 0.148148 L_1^3 + 1.16286 L_\mu + L_1 L_\mu \\ &+ (1/3) L_1^2 L_u - 0.407407_\mu^2 - (2/9) L_1 L_\mu^2 \\ &+ 0.037037 L_\mu^3 + 0.0542857 L_2 \\ &+ (1/9) L_1 L_2 + (1/9) L_1^2 L_2 \\ &- 0.185185 L_\mu L_2 - (2/9) L_1 L_\mu L_2 \\ &+ (1/9) L_\mu^2 L_2 + 0.037037 L_2^2]. \end{aligned} \tag{A4e}$$


[1] M. Peter, Phys. Rev. Lett. **78**, 602 (1997); Nucl. Phys. **B501**, 471 (1997).
[2] Y. Schröder, Phys. Lett. B **447**, 321 (1999); Nucl. Phys. B (Proc. Suppl.) **86**, 525 (2000).
[3] B.A. Kniehl, A.A. Penin, V.A. Smirnov, and M. Steinhauser, Nucl. Phys. **B635**, 357 (2002).
[4] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Phys. Rev. D **60**, 091502 (1999).
[5] B.A. Kniehl and A.A. Penin, Nucl. Phys. **B563**, 200 (1999).
[6] R. Tarrach, Nucl. Phys. **B183**, 384 (1981).
[7] N. Gray, D.J. Broadhurst, W. Grafe, and K. Schilcher, Z. Phys. C **48**, 673 (1990); L.V. Avdeev and M.Y. Kalmykov, Nucl. Phys. **B502**, 419 (1997).
[8] K.G. Chetyrkin and M. Steinhauser, Nucl. Phys. **B573**, 617 (2000); K. Melnikov and T.v. Ritbergen, Phys. Lett. B **482**, 99 (2000).
[9] A.H. Hoang, M.C. Smith, T. Stelzer, and S. Willenbrock, Phys. Rev. D **59**, 114014 (1999).
[10] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Nucl. Phys. **B566**, 275 (2000).
[11] M. Beneke, Phys. Lett. B **434**, 115 (1998).
[12] M. Neubert and C.T. Sachrajda, Nucl. Phys. **B438**, 235 (1995); M.E. Luke, A.V. Manohar, and M.J. Savage, Phys. Rev. D **51**, 4924 (1995); A.G. Grozin and M. Neubert, Nucl. Phys. **B508**, 311 (1997); F. Campanario, A.G. Grozin, and T. Mannel, *ibid.* **B663**, 280 (2003); **B670**, 331(E) (2003).
[13] A. Pineda, J. High Energy Phys. **06**, 022 (2001).
[14] T. Lee, J. High Energy Phys. **10**, 044 (2003).
[15] I.I. Bigi, M.A. Shifman, N.G. Uraltsev, and A.I. Vainshtein, Phys. Rev. D **50**, 2234 (1994).
[16] A.H. Hoang, Z. Ligeti, and A.V. Manohar, Phys. Rev. Lett. **82**, 277 (1999); Phys. Rev. D **59**, 074017 (1999).
[17] O.I. Yakovlev and S. Groote, Phys. Rev. D **63**, 074012 (2001).
[18] T. Lee, Phys. Rev. D **67**, 014020 (2003).
[19] I. Caprini and J. Fischer, Phys. Rev. D **60**, 054014 (1999).
[20] G. Cvetič and T. Lee, Phys. Rev. D **64**, 014030 (2001); G. Cvetič, T. Lee, and I. Schmidt, Phys. Lett. B **520**, 222 (2001).
[21] N.N. Khuri, Phys. Lett. **82B**, 83 (1979); C.N. Lovett-Turner and C.J. Maxwell, Nucl. Phys. **B452**, 188 (1995); P. Ball, M. Beneke, and V.M. Braun, *ibid.* **B452**, 563 (1995).
[22] G. Cvetič, Phys. Rev. D **67**, 074022 (2003).
[23] M. Beneke and V.M. Braun, Nucl. Phys. **B426**, 301 (1994).
[24] M. Beneke, Phys. Rep. **317**, 1 (1999).
[25] M. Beneke, Phys. Lett. B **344**, 341 (1995).
[26] P.M. Stevenson, Phys. Rev. D **23**, 2916 (1981).
[27] G. Cvetič, Phys. Lett. B **486**, 100 (2000); G. Cvetič and R. Kögerler, Phys. Rev. D **63**, 056013 (2001).
[28] O.V. Tarasov, A.A. Vladimirov, and A.Y. Zharkov, Phys. Lett. **93B**, 429 (1980); S.A. Larin and J.A. Vermaseren, Phys. Lett. B **303**, 334 (1993).
[29] T. van Ritbergen, J.A. Vermaseren, and S.A. Larin, Phys. Lett. B **400**, 379 (1997).
[30] J.R. Ellis, I. Jack, D.R. Jones, M. Karliner, and M.A. Samuel, Phys. Rev. D **57**, 2665 (1998).

[31] V. Elias, T.G. Steele, F. Chishtie, R. Migneron, and K.B. Sprague, Phys. Rev. D **58**, 116007 (1998).
[32] T. Lee, Phys. Rev. D **56**, 1091 (1997); T. Lee, Phys. Lett. B **462**, 1 (1999).
[33] G. Cvetič, hep-ph/0309262.
[34] G. Cvetič, C. Dib, T. Lee, and I. Schmidt, Phys. Rev. D **64**, 093016 (2001).
[35] A.A. Penin and M. Steinhauser, Phys. Lett. B **538**, 335 (2002).
[36] W. Fischler, Nucl. Phys. **B129**, 157 (1977); A. Billoire, Phys. Lett. **92B**, 343 (1980); for an application of a nonperturbative method see P. Gaete, Phys. Lett. B **515**, 382 (2001).
[37] T. Appelquist, M. Dine, and I.J. Muzinich, Phys. Rev. D **17**, 2074 (1978).
[38] B.A. Kniehl, A.A. Penin, M. Steinhauser, and V.A. Smirnov, Phys. Rev. D **65**, 091503(R) (2002).
[39] S.N. Gupta and S.F. Radford, Phys. Rev. D **24**, 2309 (1981); **25**, 3430 (1982).
[40] S. Titard and F.J. Yndurain, Phys. Rev. D **49**, 6007 (1994); A. Pineda and F.J. Yndurain, *ibid.* **58**, 094022 (1998); **61**, 077505 (2000).
[41] A. Czarnecki and K. Melnikov, Phys. Rev. Lett. **80**, 2531 (1998); Phys. Rev. D **65**, 051501(R) (2002); A.H. Hoang and T. Teubner, *ibid.* **58**, 114023 (1998); J.H. Kühn, A.A. Penin, and A.A. Pivovarov, Nucl. Phys. **B534**, 356 (1998).
[42] K. Melnikov and A. Yelkhovsky, Phys. Rev. D **59**, 114009 (1999).
[43] A.A. Penin and A.A. Pivovarov, Phys. Lett. B **435**, 413 (1998); Nucl. Phys. **B549**, 217 (1999).
[44] F.A. Chishtie and V. Elias, Phys. Lett. B **521**, 434 (2001).
[45] M. Beneke and V.A. Smirnov, Nucl. Phys. **B522**, 321 (1998); V.A. Smirnov, Phys. Lett. B **465**, 226 (1999).
[46] Y. Kiyo and Y. Sumino, Phys. Lett. B **496**, 83 (2000); Phys. Rev. D **67**, 071501(R) (2003).
[47] S. Recksiegel and Y. Sumino, Phys. Lett. B **578**, 369 (2004); Phys. Rev. D **67**, 014004 (2003).
[48] G. Cvetič and R. Kögerler, Phys. Rev. D **66**, 105009 (2002).
[49] K. Kajantie, M. Laine, K. Rummukainen, and Y. Schroder, Phys. Rev. D **67**, 105008 (2003); J.P. Blaizot, E. Iancu, and A. Rebhan, *ibid.* **68**, 025011 (2003).
[50] U. Aglietti and Z. Ligeti, Phys. Lett. B **364**, 75 (1995).
[51] K.G. Chetyrkin, B.A. Kniehl, and M. Steinhauser, Phys. Rev. Lett. **79**, 2184 (1997).
[52] G. Grunberg, Phys. Lett. **95B**, 70 (1980); **110B**, 501(E) (1982); **114B**, 271 (1982); Phys. Rev. D **29**, 2315 (1984); A.L. Kataev, N.V. Krasnikov, and A.A. Pivovarov, Nucl. Phys. **B198**, 508 (1982); A. Dhar and V. Gupta, Phys. Rev. D **29**, 2822 (1984); V. Gupta, D.V. Shirkov, and O.V. Tarasov, Int. J. Mod. Phys. A **6**, 3381 (1991).
[53] M.B. Voloshin, Nucl. Phys. **B154**, 365 (1979); H. Leutwyler, Phys. Lett. **98B**, 447 (1981); M.B. Voloshin, Sov. J. Nucl. Phys. **36**, 143 (1982) [Yad. Fiz. **36**, 247 (1982)].
[54] B.L. Ioffe and K.N. Zyablyuk, Eur. Phys. J. C **27**, 229 (2003).
[55] N. Brambilla, Y. Sumino, and A. Vairo, Phys. Rev. D **65**, 034001 (2002).
[56] D. Eiras and J. Soto, Phys. Lett. B **491**, 101 (2000).
[57] A.H. Hoang, hep-ph/0008102.
[58] Particle Data Group Collaboration, K. Hagiwara *et al.*, Phys. Rev. D **66**, 010001 (2002), and 2003 partial update for edition 2004 (URL: http://pdg.lbl.gov).
[59] V.S. Fadin and V.A. Khoze, JETP Lett. **46**, 525 (1987) [Pis'ma Zh. Eksp. Teor. Fiz. **46**, 417 (1987)].
[60] A.H. Hoang *et al.*, EPJdirect C **2**, 3 (2000).
[61] A.A. Penin and A.A. Pivovarov, Nucl. Phys. **B550**, 375 (1999); Phys. At. Nucl. **64**, 275 (2001) [Yad. Fiz. **64**, 323 (2001)].
[62] M. Böhm, H. Spiesberger, and W. Hollik, Fortschr. Phys. **34**, 687 (1986); F. Jegerlehner, M.Y. Kalmykov, and O. Veretin, Nucl. Phys. **B658**, 49 (2003).
[63] F. Jegerlehner and M.Y. Kalmykov, hep-ph/0308216.
[64] B.V. Geshkenbein, B.L. Ioffe, and K.N. Zyablyuk, Phys. Rev. D **64**, 093009 (2001).
[65] ALEPH Collaboration, R. Barate *et al.*, Eur. Phys. J. C **4**, 409 (1998).
[66] S. Bethke, Nucl. Phys. B (Proc. Suppl.) **121**, 74 (2003).
[67] M. Beneke and A. Signer, Phys. Lett. B **471**, 233 (1999).
[68] J.H. Kühn and M. Steinhauser, Nucl. Phys. **B619**, 588 (2001); **B640**, 415(E) (2002).
[69] G. Corcella and A.H. Hoang, Phys. Lett. B **554**, 133 (2003).
[70] M. Eidemüller, Phys. Rev. D **67**, 113002 (2003).
[71] A.H. Hoang and T. Teubner, Phys. Rev. D **60**, 114027 (1999).
[72] K. Melnikov and A. Yelkhovsky, Nucl. Phys. **B528**, 59 (1998).
[73] O.I. Yakovlev, Phys. Lett. B **457**, 170 (1999).
[74] T. Nagano, A. Ota, and Y. Sumino, Phys. Rev. D **60**, 114014 (1999).