Calculation of binding energies and masses of quarkonia in analytic QCD models

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(Dated: May 10, 2014)

We extract quark masses \( m_q \) (\( q = b, c \)) from the evaluation of the masses of quarkonia \( Y(1S) \) and \( J/\psi(1S) \), performed in two analytic QCD models, and in perturbative QCD in two renormalization schemes. In analytic QCD the running coupling has no unphysical singularities in the low-momentum regime. We apply the analytic model of Shirkov et al. [Analytic Perturbation Theory (APT)], extended by Bakulev et al. [Fractional Analytic Perturbation Theory (FAPT)], and the two-delta analytic model (2\( \delta \)anQCD). The latter, in contrast to (F)APT, at higher energies basically coincides with the perturbative QCD (in the same scheme). We use the renormalon-free mass \( \bar{m}_q \) as input. The separation of the soft and ultrasoft parts of the binding energy \( E_{\bar{q}q} \) is performed by the requirement of the cancellation of the leading infrared renormalon. The analysis in the 2\( \delta \)anQCD model indicates that the low-momentum ultrasoft regime is important for the extraction of the masses \( \bar{m}_q \), especially \( \bar{m}_b \). The 2\( \delta \)anQCD model gives us clues on how to estimate the influence of the ultrasoft sector on \( m_q \) in general. These effects lead to relatively large values \( \bar{m}_s \approx 4.35 \pm 0.08 \) GeV in the 2\( \delta \)anQCD model, which, however, are compatible with recent lattice calculations. In perturbative QCD in MS scheme these effects are even stronger and give larger uncertainties in \( \bar{m}_s \). The (F)APT model gives small ultrasoft effects and the extracted values of \( \bar{m}_s \) agree with those in most of the literature (\( \bar{m}_s \approx 4.2 \) GeV). The extracted values of \( \bar{m}_c \) in all four models are about 1.26-1.27 GeV and agree well with those in the literature.

PACS numbers: 12.38.Cy, 12.38.Aw,12.40.Vv

I. INTRODUCTION

Most of the calculations of the masses of heavy quarkonia are based on perturbative expansions. These expansions come from the knowledge of the static quark-antiquark potential \( V(r) \) which has been calculated up to N\( ^3 \)LO (\( \sim \alpha_s^3/r \)) in Refs. [1,2]. At N\( ^3 \)LO (\( \sim \alpha_s^3/r \)) level, ultrasoft gluons contribute to \( V(r) \) and the calculation of these terms has been completed in Refs. [3,6]. The expansion coefficients for the mass of the (heavy) \( q\bar{q} \) quarkonium vector \( (S = 1) \) or scalar \( (S = 0) \) ground state (i.e., with: \( n = 1 \) and \( \ell = 0 \)) are given, for example, in Ref. [7], for the terms including \( m_q \alpha_s^5 \). The latter term is known because the potential \( V(r) \) is known at \( \sim \alpha_s^2/r \) level. For a review of the topic, see, e.g. Ref. [8].

Most of the radiative contributions to the quarkonium mass expansion are from the so called soft sector of gluon momenta, \( Q \sim m_q \alpha_s \). In the cases of \( b\bar{b} \) and \( c\bar{c} \), these are around 2 GeV and 1 GeV, respectively. At \( Q \approx 2 \) GeV scales, the perturbative QCD (pQCD) coupling \( \alpha_s(Q^2) \) is marginally reliable; at \( Q \approx 1 \) GeV it is unreliable. This is so because the pQCD coupling \( \alpha_s(Q^2) \) suffers from unphysical (Landau) singularities at low spacelike \( q^2 \) (\( \equiv -Q^2 \)), i.e., at \( 0 < Q^2 < \Lambda^2 \) where \( \Lambda^2 \approx 10^{-1} \) GeV\(^2 \); for \( Q^2 \approx 1 \) GeV\(^2 \) it is dangerously close to these singularities, and thus unreliable.

The aforementioned Landau singularities are not physical because they do not possess the analytic properties of the spacelike observables \( D(Q^2) \) (such as the Adler function), the latter properties being dictated by the general properties of quantum field theories [9,10] including causality. Namely, \( D(Q^2) \) must be an analytic function in the entire complex \( Q^2 \) plane, with the exception of the timelike semiaxis \( Q^2 < -M_{th}^2 \), where \( M_{th} \sim 10^{-1} \) GeV is a particle production threshold. Specifically, the evaluation of spacelike quantities \( D(Q^2) \) in pQCD, as a (truncated) power series of the perturbative running coupling (couplant) \( \alpha_s(\kappa Q^2) \equiv \alpha_s(\kappa^2)/\pi \) (with \( \kappa \sim 1 \)), does not respect these important analytic properties of \( D(Q^2) \). These problems, within the context of QCD, were first addressed in the seminal works

† In comparison with v1: improved presentation; (F)APT calculation performed in the \( \beta_2 = \beta_3 = \cdots = 0 \) scheme; comparison with the results of other methods in the literature included (cf. Table IV); part of the text moved into the new Appendix A; the basic conclusions unchanged; extended acknowledgments: Refs. [12,38-39,41,44,80-83,89-99,110-11] are new.

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1 The momentum transfer \( q \) of the gluon is spacelike, i.e., \( q^2 \equiv -Q^2 < 0 \), because the scattering of the quark and antiquark in the quarkonium is of the \( t \)-channel type.
of Shirkov, Solovtsov, Milton et al. \[11\]-\[16\]. There, the perturbative running coupling $a_{pt}(Q^2) \equiv \alpha_s(Q^2)/\pi$ was made an analytic (in the aforementioned sense) function of $Q^2$, $a_{pt}(Q^2) \rightarrow A_1^{(APT)}(Q^2)$, in the following way: in the dispersion relation the discontinuity function $\rho_1^{(pt)}(\sigma) \equiv \text{Im } a_{pt}(Q^2 = -\sigma - i\epsilon)$ was kept unchanged on the entire negative axis in the complex $Q^2$-plane (i.e., for $\sigma \geq 0$), and was set equal to zero on the nonphysical cut $0 < Q^2 < \Lambda^2$. For this reason, this analytic QCD (anQCD) model can be referred to as the minimal analytic (MA) model. Here we will refer to this model by its usual name used in the literature: Analytic Perturbation Theory (APT).

Various other analytic QCD (anQCD) models for $A_1(Q^2)$ can be constructed, and have been presented in the literature, among them Refs. \[17\]-\[25\]. These models fulfill certain additional constraints at low and/or at high $Q^2$. For further literature on various analytic QCD models, we refer to the review articles in Refs. \[26\]-\[29\]. Some newer constructions of anQCD models of \[36\], \[37\]. The latter basically states that the terms in OPE of higher dimension ($D > 8$) need to modify the ITEP school (Institute of Theoretical and Experimental Physics) interpretation of the OPE of the corresponding (in the scheme) pQCD coupling: $A_1^{(APT)}(Q^2)$ including terms of dimension $D \leq 8$ without the need to modify the ITEP school (Institute of Theoretical and Experimental Physics) interpretation of the OPE \[36\], \[37\]. The latter basically states that the terms in OPE of higher dimension ($D > 0$) originate from the infrared regime only.

Once we have an anQCD model, i.e., a model for the analytic analog $A_1(Q^2)$ of the pQCD coupling $a_{pt}(Q^2)$ (or, equivalently, for the discontinuity function $\rho_1(\sigma)$), the analytic analogs $A_n(Q^2)$ of the higher powers $a_{pt}(Q^2)^n$ have to be constructed from $A_1(Q^2)$. In the case of APT ($A_1^{(APT)}(Q^2)$), for integer $n$, the couplings $A_n^{(APT)}(Q^2)$ were constructed in Refs. \[12\], \[14\]. However, perturbation expansions of some observables, and effects of evolution of distribution amplitudes at a chosen loop-level, are represented sometimes by noninteger powers $a_{pt}(Q^2)^\nu$ or logarithmic terms $a_{pt}(Q^2)^\nu \ln^k a_{pt}(Q^2)$ ($\nu$ noninteger, $k$ integer). Among them are the pion electromagnetic form factor $F_\pi(Q^2)$ and hadronic decay width of Higgs $\Gamma_{H \rightarrow b\bar{b}}$. The problems of the analytization of such quantities, within the spirit of APT, were considered in Ref. \[38\], where the dispersion relations were extended from the coupling parameter to the general QCD amplitudes. The APT approach to evaluation of the (factorizable part) of the form factor $F_\pi(Q^2)$ was performed in Ref. \[59\], where the nonperturbative distribution amplitude was evaluated by performing numerical evolution with an analytic coupling parameter. The authors Bakulev, Mikhailov and Stefanis (BMS) then systematically extended APT in Ref. \[40\] to the evaluation of noninteger power analogs $A_n(Q^2)$ and $A_{n,k}(Q^2)$ of the mentioned terms $a_{pt}(Q^2)^\nu$ and $a_{pt}(Q^2)^\nu \ln^k a_{pt}(Q^2)$. This extension was performed for the spacelike quantities, with explicit expressions at the one-loop level, and extension to the higher-loop level via expansions of the one-loop expressions. This was then applied to an evaluation of the factorizable part of $F_\pi(Q^2)$ in Ref. \[41\]. In Ref. \[42\] the authors extended this construction to the timelike quantities and applied it to the evaluation of the Higgs decay width $\Gamma_{H \rightarrow b\bar{b}}(s)$ in APT. In Ref. \[43\] this construction was applied to the evaluation of the $e^+e^- \rightarrow$ hadrons ratio $R$, and a detailed analysis of the calculation of $\Gamma_{H \rightarrow b\bar{b}}$ in APT. In the review work of Bakulev, Ref. \[29\], several variants of this construction are reviewed, among them the numerical dispersive approach at the two-loop and higher-loop level (Secs. III B, C, D of Ref. \[29\]); a mathematical package for such numerical calculation is given in Ref. \[44\]. The construction of BMS is referred to in the literature as the Fractional Analytic Perturbation Theory (FAPT).

In the general case of analytic $A_1(Q^2)$, the quantities $A_n(Q^2)$ were constructed in Refs. \[22\]-\[29\] for integer $n$, as linear combinations of logarithmic derivatives $A_k(Q^2) \propto d^{k-1}A_1(Q^2)/d(\ln Q^2)^{k-1}$ ($k \geq n$), and were extended to noninteger $n$ in Ref. \[46\].

In this work, we apply two anQCD models of $(a_{pt})_{an} \equiv A_1$, namely APT of Refs. \[11\]-\[16\], and the $2\delta$anQCD model of Refs. \[34\], \[35\], to evaluations of the perturbation series of the binding energy $E_{q\bar{q}}$ of heavy quarkonia $(\Upsilon(1S)$ and $J/\psi(1S))$ and of the quark pole mass $m_q$. In this way, we will evaluate the masses of these quarkonia $M_{q\bar{q}} = 2m_q + E_{q\bar{q}}$ as functions of the (MS) quark mass $m_q$. In the APT model of analytic QCD (i.e., the model for $A_1^{(APT)}(Q^2)$, Ref. \[11\]), we will need to evaluate not just the integer power analogs $(a_{pt}^n)_{an, APT} \equiv A_n^{(APT)}(Q^2)$, but also the analogs of the logarithmic terms $(a_{pt}^n \ln^k a_{pt})_{an, APT}$, whose evaluation uses the approach of FAPT.

\[2\] The relations between such functions $A_k$’s and $A_n$’s, allowing a recurrent construction of $A_n$, for integer $n$ within the context of the APT model, were given also in Refs. \[27\]-\[45\].
As input parameter we use the renormalon-free quark mass $\overline{m}_q (\equiv \overline{m}_q (\mu^2 = m_q^2))$ of the corresponding quark $q = b, c$ (also called the $\overline{MS}$ quark mass), and the anQCD coupling of the model. Since the quarkonia masses are well measured, we can extract the values of $\overline{m}_q$. We also perform the same analysis in pQCD in the corresponding renormalization schemes.

In Sec. II we briefly describe the (F)APT model (Sec. II A) and the $2\delta$anQCD model (Sec. II B). In Sec. III we present the procedures of evaluation of the binding energy $E_q^\overline{q}$ and of the quark pole mass $m_q$, in terms of the mass $\overline{m}_q$ and of the couplings. Furthermore, we explain how the cancellation of the leading infrared renormalon in the sum $2m_q + E_q^\overline{q}$ allows us to separate the ultrasoft from the soft part of the binding energy. The numerical results and the extractions of the masses $\overline{m}_b$ and $\overline{m}_c$ are presented in Sec. IV (Secs. IV A and IV B respectively). The evaluations are performed in the two aforementioned analytic models (F)APT and $2\delta$anQCD, and in pQCD in the corresponding two renormalization schemes ($\overline{MS}$, and in the scheme of $2\delta$anQCD called here the Lambert scheme). In Sec. V we summarize our results and draw certain conclusions. Appendix A summarizes the construction of the higher order analytic analogs $A_\nu$ for the powers $a_\nu^\mu$, and for the logarithmic-type terms $a_\nu^\mu \ln^k a_\nu$, for general $\nu$ and integer $k$, in general anQCD models. Appendix B contains the expressions of the coefficients of the perturbation expansion of $E_q^\overline{q}$, available from the literature. Appendix C contains a renormalon-based estimation of the coefficient at the $a_\nu^\mu$ term in the perturbation expansion of $m_q/\overline{m}_q$. Appendix D has some useful formulas for the scale and scheme dependence of $a_\nu$.

II. TWO ANALYTIC QCD MODELS

A. (Fractional) Analytic Perturbation Theory

As already mentioned in the Introduction, the coupling $a_\nu (Q^2) \equiv \alpha_\nu (Q^2)/\pi$ in pQCD in the usual renormalization schemes (such as $\overline{MS}$, or the $\beta_2 = \beta_3 = \ldots = 0$ scheme), possesses unphysical (Landau) singularities inside the required analyticity regime $Q^2 \in C \setminus (-\infty, 0]$. Specifically, it has a cut on the semiaxis $(-\infty, \Lambda_2^2)$, (where $\Lambda_2^2 \sim 10^{-11}$ GeV$^2$ is the “Landau” branching point), thus offending the analyticity requirement on the cut sector $Q^2 \in (0, \Lambda_2^2)$. Application of the Cauchy theorem gives us the following dispersion relation:

$$a_\nu^\mu (Q^2) = \frac{1}{\pi} \int_{\sigma=-\Lambda_2^2}^{\infty} \frac{d\sigma}{\sigma + Q^2} \Im a_\nu^\mu (\sigma - i\epsilon).$$

We also perform the same procedure as in pQCD in the corresponding $\overline{MS}$ scheme of $2\delta$anQCD, and in pQCD in the corresponding two renormalization schemes ($\overline{MS}$, and in the scheme of $2\delta$anQCD called here the Lambert scheme). In Sec. V we summarize our results and draw certain conclusions. Appendix A summarizes the construction of the higher order analytic analogs $A_\nu$ for the powers $a_\nu^\mu$, and for the logarithmic-type terms $a_\nu^\mu \ln^k a_\nu$, for general $\nu$ and integer $k$, in general anQCD models. Appendix B contains the expressions of the coefficients of the perturbation expansion of $E_q^\overline{q}$, available from the literature. Appendix C contains a renormalon-based estimation of the coefficient at the $a_\nu^\mu$ term in the perturbation expansion of $m_q/\overline{m}_q$. Appendix D has some useful formulas for the scale and scheme dependence of $a_\nu$. 

In evaluation of general spacelike observables in pQCD, terms of the type $a_\nu^\mu (Q^2) \ln^k a_\nu (Q^2)$ may appear, with $\nu > 0$ and (nonnegative) integers $k$ and $\ell$. In APT, in principle, the factor $\ln\frac{Q^2}{m^2}$ may be included in the FAPT-type analytization (see, for example, Ref. [29]). However, the factor $\ln\frac{Q^2}{m^2}$ is analytic function in the complex $Q^2$ plane with the exclusion of the nonpositive axis $Q^2 \leq 0$. On the other hand, this is also the regime of analyticity of $A_1^{\text{APT}} (Q^2)$ [note that $Q^2 = 0$ is a point of nonanalyticity of $A_1^{\text{APT}} (Q^2)$ because $dA_1^{\text{APT}} (Q^2)/dQ^2 = \infty$ there]. Therefore, we will not include the factor $\ln\frac{Q^2}{m^2}$ in the (FAPT)-type analytization. With these considerations, all the other pQCD terms in such observables, $a_\nu^\mu (Q^2) \ln^k a_\nu (Q^2)$, are made analytic in (F)APT by the same procedure as $a_\nu^\mu (Q^2)$ in Eq. (2):

$$\left( a_\nu^\mu (Q^2) \ln^k a_\nu (Q^2) \right)^{(\text{FAPT})}_{\text{an}} \equiv A_{\nu,k}^{\text{(FAPT)}} (Q^2) = \frac{1}{\pi} \int_{\sigma=0}^{\infty} \frac{d\sigma}{\sigma + Q^2} \Im \left[ a_\nu^\mu (\sigma - i\epsilon) \ln^k a_\nu (\sigma - i\epsilon) \right].$$

In this context, the authors of Refs. [29, 30, 42, 43] derived explicit simple formulas for these minimal analytic expressions at one-loop level, and the related more involved expressions at higher-loop levels — expressions from which the analyticity structure in $Q^2$ and in $\nu$ can be more clearly seen. For our calculational purposes, though, the dispersion formulas (5) will be applied, numerically, when the (F)APT model is used, in the same spirit as was performed by Bakulev in Ref. [29] (Sec. III C there), and in Ref. [44].
APT has a relatively specific and interesting property, namely, that the couplings differ from the corresponding pQCD couplings in a nonnegligible way even at high $|Q^2|$ 

$$A_1^{(\text{APT})}(Q^2) - a_{\text{pt}}(Q^2) \sim \Lambda^2 / Q^2 \quad (|Q^2| > \Lambda^2) .$$

(4)

As a consequence, $A_n^{(\text{APT})}(Q^2)$ and $a_{\text{pt}}(Q^2)^n$ differ from each other in a nonnegligible way even at high $|Q^2|$ [10]; we cannot approximate $A_1^{(\text{APT})}(Q^2)$ well with $a_{\text{pt}}(Q^2)$ even at as high $|Q^2|$ as $\sim M_Z^2$. The (only) free parameter in APT is the $\overline{\text{MS}}$ scale $\Lambda$, which appears in the usual perturbation expansion of the underlying pQCD coupling $a_{\text{pt}}(Q^2; \overline{\text{MS}})$ in inverse powers of $\ln(Q^2/\Lambda^2)$ [i.e., the $a_{\text{pt}}$ whose discontinuity functions appear in the relations (2)-(3)].

We will consider that in APT this scale varies in the interval $\overline{\Lambda}_{N_f=5} = 0.260\pm 0.030$ GeV. The analysis of high-energy QCD observables (with $|Q| \gtrsim 10^4$ GeV) in Ref. [16] suggests a value of $\overline{\Lambda}_{N_f=5} \approx 0.290$ GeV [corresponding to $\alpha_s(M_Z^2; \overline{\text{MS}}) \approx 0.124$]. The works of Refs. [29 42 43] use the value $\overline{\Lambda}_{N_f=5} \approx 0.260$ GeV instead [corresponding to $\alpha_s(M_Z^2; \overline{\text{MS}}) \approx 0.122$ and giving the timelike (Minkowskian) coupling $\Lambda_1(M_Z^2) \approx 0.120$]. On the other hand, if the “average” $e^+e^-$ annihilation ratio $R(s)$ value at $\sqrt{s} = M_Z$ is taken to be $\approx 1.03904$ as used, e.g., in Ref. [17], (F)APT approach of evaluating $R(M_Z^2)$ gives $\overline{\Lambda}_{N_f=5} \approx 0.225$ GeV [48].

In comparison, pQCD analyses give for $\alpha_s(M_Z^2)$ the world average $0.1184\pm 0.0007$ [49], corresponding to $\overline{\Lambda}_{N_f=5} = 0.213\pm 0.008$ GeV, i.e., significantly lower scales than for APT.3

Due to the nonnegligible difference, Eq. (4), the threshold effects of heavy quarks have to be implemented in APT. This is performed by requiring the continuity of the perturbative coupling [whose discontinuities are used in APT]

$$a_{\text{pt}}(Q^2) = f_{N_f}(Q^2/\overline{\Lambda}_{N_f}^2) ,$$

(5)

at positive “threshold” values $Q^2 = Q_{N_f-1\rightarrow N_f}^2 > 0$ chosen to be for $N_f = 4, 5, 6$ the squares of the current heavy quark masses $m_c \equiv m_4$, $m_b \equiv m_5$ and $m_t \equiv m_6$, respectively [16]

$$f_{N_f-1}(m_{N_f-1}/\overline{\Lambda}_{N_f-1}^2) = f_{N_f}(m_{N_f}/\overline{\Lambda}_{N_f}^2) \quad (N_f = 4, 5, 6) .$$

(6)

Further, it is assumed that, for complex $Q^2$, the values of $a_{\text{pt}}(Q^2)$ involve the scale $\overline{\Lambda}_{N_f}$ determined by the absolute value $|Q^2|$ 

$$a_{\text{pt}}(Q^2) = f_{N_f}(Q^2/\overline{\Lambda}_{N_f}^2) \quad \text{for}: \quad m_{N_f}^2 < |Q^2| < m_{N_f+1}^2 .$$

(7)

Thus constructed $a_{\text{pt}}(Q^2)$ gives the piecewise discontinuous global APT discontinuity functions. For example, for $\rho_{\nu,k}^{(\text{pt})}(\sigma) \equiv \text{Im}[a_{\text{pt}}(\ln k a_{\text{pt}}(-\sigma - i\epsilon))]$, this globalization results in

$$\rho_{\nu,k}^{(\text{pt})}(\sigma) \equiv \text{Im} \left( a_{\text{pt}}(\ln k a_{\text{pt}}(-\sigma - i\epsilon)) \right) = \text{Im} \left[ f_{N_f}(z)^\nu \ln k f_{N_f}(z) \right] \bigg|_{z=-\sigma/\overline{\Lambda}_{N_f}^2 - i\epsilon} \quad \text{for}: \quad (m_{N_f}^2 < \sigma < m_{N_f+1}^2) .$$

(8)

Despite the discontinuity of $\rho_{\nu,k}^{(\text{pt})}(\sigma)$, the (F)APT analytic analogs [3] are analytic functions.

For the underlying $a_{\text{pt}}(Q^2) \equiv \alpha_s(Q^2)/\pi$ we will use the coupling in the $\beta_2 = \beta_3 = \cdots = 0$ renormalization scheme [50 52], i.e., the coupling which fulfills the two-loop renormalization group equation (RGE)

$$\frac{d a_{\text{pt}}(Q^2)}{d \ln Q^2} = -\beta_0 a_{\text{pt}}^2 (1 + c_1 a_{\text{pt}}) .$$

(9)

Here, $c_1 = \beta_1/\beta_0$, the constants $\beta_0 = (1/4)(11 - 2N_f/3)$ and $\beta_1 = (102 - 38N_f/3)/16$ are universal, and the scale $Q^2$ is complex in general, $Q^2 = |Q^2| \exp(i\phi)$. This equation has an explicit solution of the form [50 52]

$$a_{\text{pt}}(Q^2) = -\frac{1}{c_1 \left[ 1 + W_{+1}(z) \right]} ,$$

(10)

3 Also the anQCD models of Refs. [17 18] differ nonnegligibly from pQCD, even at high $|Q^2|$.
$W_{-1}$ and $W_{+1}$ are the branches of the Lambert function for the case $0 \leq \phi < +\pi$ and $-\pi < \phi < 0$, respectively, and

$$z(Q^2) = -\frac{1}{c_1 e} \left( \frac{Q^2}{\Lambda^2} \right)^{-\beta_0/c_1} \exp\left(-i\beta_0 \phi/c_1\right).$$

(11)

We call the scale $\Lambda^2$ ($\sim 0.1$ GeV$^2$) appearing here the Lambert scale. The aforementioned values $\Lambda_{N_f=5} = 0.260 \pm 0.030$ GeV, in the scheme $\beta_2 = \beta_3 = \cdots = 0$, correspond to $\Lambda_{N_f=5} = 0.322 \pm 0.037$ GeV. The solution (10) is convenient because it represents an explicit function$^4$ and it is thus easy to evaluate it and the corresponding discontinuity functions $\rho_{n,k}^{(an)}(\sigma)$, Eq. (3), in practice. It has Landau singularities.

Using the aforementioned value $\Lambda_5 = 0.322 \pm 0.037$ GeV ($\Lambda_5 = 0.260 \pm 0.030$ GeV), the continuity conditions (6) give us at other values of $N_f$: $\Lambda_1 = 0.476 \pm 0.050$ GeV ($\Lambda_1 = 0.366 \pm 0.038$ GeV), $\Lambda_3 = 0.581 \pm 0.055$ GeV ($\Lambda_3 = 0.427 \pm 0.040$ GeV), and $\Lambda_6 = 0.128 \pm 0.016$ GeV ($\Lambda_6 = 0.110 \pm 0.014$ GeV). The first three quark flavors are regarded to be massless.

In this context, we mention that the elimination of the Landau singularities (i.e., analytization) of $a_{pt}(Q^2)$ can be performed in various ways, not just in the “minimal” way of Eq. (2). This analytization, in general results in an (analytic) running coupling $A_1(Q^2)$ which differs from the corresponding perturbative one by a power term

$$A_1(Q^2) = a_{pt}(Q^2) + O\left( \left( \frac{\Lambda^2}{Q^2} \right)^n \right), \quad (|Q^2| > \Lambda^2).$$

(12)

In the case of APT, the power index is $n = 1$, cf. Eq. (1). This index can be increased to $n = 3$ [19] [33], and even to $n = 5$ [34], while still maintaining analyticity. In Refs. [31] [32] the problem of finding perturbative analytic couplings (in specific schemes) was investigated. It turned out that such couplings always gave a value of the (strangeless) semihadronic tau lepton decay ratio $r$, that was significantly too low, unless the scheme was changed in a drastic way which made the perturbation series diverge strongly after the first four terms.

Therefore, the appearance of the power terms as given in Eq. (12) seems to be a general feature of procedures which eliminate the unphysical (Landau) singularities of the coupling in the complex $Q^2$-plane. These power terms are of ultraviolet origin and thus contravene the philosophy of the ITEP school [30], according to which the power terms in (inclusive) QCD observables appear in the OPE and are of infrared origin. Furthermore, in APT we have $n = 1$ and the terms $\sim \Lambda^2/Q^2$ appear even in the massless QCD, i.e., in the case when such terms are not allowed in the usual pQCD+OPE approach for observables related with the vacuum expectation values (such as the Adler function). In general, the ITEP interpretation of the OPE must be abandoned in those anQCD models in which the index $n$ in Eq. (12) is low (e.g., $n \leq 2$), and modified or restricted in others (e.g., when $n = 3, 4$).$^5$

We evaluate quarkonium masses with the (F)APT model of anQCD, illustrating the effects of elimination of Landau singularities on the behavior of the series. The (F)APT model is relatively simple to apply technically.

We will also apply another anQCD model to the evaluation of quarkonium masses, namely the so called two-delta anQCD (2δanQCD) [34], in which the index in Eq. (12) is $n = 5$. Evaluations in such models are technically more demanding, though, because the evaluation of the analytic analogs of noninteger powers $a_{pt}^\nu$ and of the logarithm-type terms $a^\nu \ln^k a$ is more involved [36].

### B. Two-delta analytic QCD model (2δanQCD)

It is possible to construct such anQCD models which, at high momenta, practically merge with pQCD; namely, with the analytic coupling $A_1(Q^2)$ which fulfills Eq. (12) with $n > 1$. One such model, with $n = 3$, was constructed in Ref. [19].$^6$ Another such anQCD model, which we can call the one-delta model, was constructed in Ref. [33], and also satisfies Eq. (12) with $n = 3$. The idea was simple: the perturbative discontinuity function $\rho_n^{(pt)}(\sigma) \equiv \text{Im } a_{pt}(Q^2 = -\sigma - i\epsilon)$, for $\sigma > 0$, was kept unchanged for $\sigma$ down to a “pQCD-onset-scale” $M_0^2 \sim 1$ GeV$^2$, and the unknown

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$^4$ In Mathematica [33] the Lambert function $W_a(z)$ is implemented under the name ProductLog[n, z].

$^5$ Nonetheless, even in APT, OPE can be applied, and has successfully been applied – see, for example, the inclusion of higher-twist terms in the APT vs pQCD analysis of the Bjorken polarized sum rule at low $Q^2$, Refs. [32]. We note that the leading-twist ($D = 0$) term, in such an APT+OPE approach, contains implicitly (parts of) the power term contributions $\sim (\Lambda^2/Q^2)^n$, $n = 1, 2, \ldots$.

$^6$ The higher couplings $A_n(Q^2) = (a_{pt}(Q^2))^n a_n$ were not constructed there, though.
low-energy regime $0 < \sigma < M_\sigma^2$ was parametrized with one delta function at a scale $M_\sigma^2$ (such that: $0 < M_\sigma^2 < M_0^2$):^7

$$\rho_1^{(18)}(\sigma) = \pi f_j^2 \Lambda^2 \delta(\sigma - M_j^2) + \Theta(\sigma - M_0^2) \times \rho_1^{pt}(\sigma),$$  

(13)

where for $a_{pt}(Q^2)$ [the latter defining $\rho_1^{pt}(\sigma)$] the renormalization scheme with $c_2 = c_3 = \ldots = 0$ was used. The (Lambert) scale parameter $\Lambda$ was fixed by the value of $\alpha_s(M_\sigma^2, \overline{\text{MS}})$. The dimensionless parameters $s_j \equiv M_j^2/\Lambda^2$ ($j = 0, 1$) and $f_k^2$ were then fixed by the requirement of $n = 3$ in Eq. (12) (these are in fact two conditions) and by the requirement that the central experimental value of the strangeless ($V + A$) $\tau$-decay ratio $r_\tau$, namely $(r_\tau)_{\exp} = 0.203 \pm 0.004$ \cite{60, 61},^8 be reproduced in the model.

As argued at the end of the previous subsection, the ITEP interpretation of the OPE requires that index $n$ in Eq. (12) be relatively high,^9 $4 < n < 9$. If, instead of one delta, we use two deltas to parametrize the otherwise unknown low-$\sigma$ regime behavior of the spectral function $\rho_1(\sigma)$, we obtain an analytic QCD model with $A_1(Q^2)$ fulfilling the relation (12) with $n = 5$, Ref. \cite{34},

$$\rho_1^{(28)}(\sigma; c_2) = \pi \sum_{j=1}^2 f_j^2 \Lambda^2 \delta(\sigma - M_j^2) + \Theta(\sigma - M_0^2) \times \rho_1^{pt}(\sigma; c_2)$$  

(14)

$$= \pi \sum_{j=1}^2 f_j^2 \delta(s - s_j) + \Theta(s - s_0) \times \rho_1^{pt}(s; c_2).$$  

(15)

Here, $s = \sigma/\Lambda^2$, and five dimensionless parameters are: $s_j = M_j^2/\Lambda^2$ ($j = 0, 1, 2$) and $f_k^2$ ($k = 1, 2$). Further, $c_2 = \beta_2/\beta_0$ is the scheme parameter, and $\rho_1^{pt}(s; c_2) = \rho_1^{pt}(\sigma; c_2) = \text{Im} a_{pt}(Q^2) = -\sigma - i\epsilon; c_2$ is the perturbative spectral function of $a_{pt}(Q^2)$ in terms of $s = \sigma/\Lambda^2$. Here $a_{pt}(Q^2)$ is given by

$$a_{pt}(Q^2) = -\frac{1}{c_1 \left[1 - c_2/c_1 + W_{+1}(z)\right]},$$  

(16)

where: $c_j \equiv \beta_j/\beta_0$ ($j = 1, 2$); $Q^2 = |Q^2| \exp(i\phi)$; and $W_{-1}$ and $W_{+1}$ are the branches of the Lambert function for the case $0 < \phi + \pi$ and $-\pi < \phi < 0$, respectively. The argument $z = z(Q^2)$ in terms of $Q^2$ is given in Eq. (11), with $\Lambda$ there being the Lambert scale. The solution (16) is the solution to the RGE where the beta function has the Padé form $\beta(a_{pt}) \propto a_{pt}^2 \times [1/1](a_{pt})$

$$\frac{da_{pt}(Q^2)}{d\ln Q^2} = -\beta_0 a_{pt}^2 \frac{[1 + (c_1 - c_2/c_1)a_{pt}]}{[1 - (c_2/c_1)a_{pt}]}.$$  

(17)

The expansion of beta function $\beta(a_{pt})$ on the right-hand side gives

$$\beta(a_{pt}) = -\beta_0 a_{pt}^2 \left(1 + c_1 a_{pt} + c_2 a_{pt}^2 + c_3 a_{pt}^3 + \ldots\right),$$  

(18)

where the higher renormalization scheme parameters $c_j$ ($j \geq 3$) are fixed by the leading scheme parameter $c_2$: $c_2 = c_2^{-1}/c_1^{-2}$. In the case of (F)APT of the previous subsection, $c_2 = 0$ was taken (effectively as two-loop running). In the case of the model in this subsection, the parameter $c_2$ will be varied in an interval, as specified below. The spacelike coupling $A_1(Q^2)$ is then obtained by the dispersion relation

$$A_1^{(24)}(Q^2) = \frac{1}{\pi} \int_{\sigma=0}^{\infty} d\sigma \rho_1^{(28)}(\sigma) = \frac{1}{\pi} \sum_{j=1}^2 \int_{s_j}^{s_j + 1} ds \rho_1^{pt}(s; c_2),$$  

(19)

where we denoted $u = Q^2/\Lambda^2$. We call this model the two-delta analytic QCD model ($2\deltaQCD$). It is to be applied in the low-momentum regime, i.e., where $N_f = 3$ (considering the current masses of $u$, $d$ and $s$ zero): $|Q^2| < (2m_c)^2$.

---

^7 A similar idea was applied in Refs. \cite{55, 56} directly to spectral functions of the vector current correlators. Other approaches of eliminating unphysical singularities directly from specific (spacelike) observables, were presented in Refs. \cite{57, 58}.

^8 $r_\tau$ is the QCD part of the $V + A$ decay ratio $R_\tau(\Delta S = 0)$, with the (small) quark mass effects subtracted. It is normalized in the canonical way: $r_\tau = a + O(a^2)$.

^9 Small-size instanton effects may lead to the conditions Eq. (12) to be valid only up to index $n$ such that $2n$ is the largest dimension of condensates not affected by the instantons. Instanton-antistanton gas scenarios lead to $n < 4\beta_0 (= 9$ for $N_f = 3$), cf. Ref. \cite{57}. 
In Ref. [34] we included the case of APT, i.e., $A_1^{\text{APT}}(Q^2)$ of Ref. [11], the analytization procedure of Appendix A is, in principle, equivalent to that of Eqs. (2)-(3), as argued in Refs. [23, 46]. The (small) differences between the two analytizations in APT arise due to somewhat different truncations applied in the two approaches. In the FAPT procedure of Eqs. (2)-(3), applicable only in APT, usually the truncation in the loop expansion ($\leq a_{pt}^{(\pm 1)}$) is applied to the running coupling $a_{pt}(\mu^2)$, which is then reflected in the spectral functions $\text{Im} a_{pt}^{(\nu)}(-\sigma - i\epsilon)$ and $\text{Im}[a_{pt}^{(\nu)}(-\sigma - i\epsilon) \ln^k a_{pt}(-\sigma - i\epsilon)]$ in Eqs. (2)-(3). In the general approach, Eqs. (A7)-(A10) of Appendix A which can be applied also to the APT analytic model of $A_1(Q^2)_{\text{APT}}$ of Ref. [11], the same kind of truncation for $a_{pt}(\mu^2)$ can be applied in $\rho_1^{(\text{pt})}(\sigma) = \text{Im} a_{pt}(Q^2 = -\sigma - i\epsilon)$, 

\begin{table}
\begin{tabular}{c|cccccccc}
$c_2 = \beta_2 / \beta_0$ & $s_0$ & $s_1$ & $f_2^2$ & $s_2$ & $f_2^2$ & $\Lambda$ [GeV] & $M_0$ & $A_1(0)$ \\
-2.10 & 17.09 & 12.523 & 0.1815 & 0.7796 & 0.3462 & 0.363 & 1.50 & 0.544 \\
-4.76 & 23.06 & 16.837 & 0.2713 & 0.8077 & 0.5409 & 0.260 & 1.25 & 0.776 \\
-5.73 & 25.01 & 18.220 & 0.3091 & 0.7082 & 0.6312 & 0.231 & 1.15 & 1.00 \\
\end{tabular}
\caption{Values of the parameters of the considered 2$\delta$anQCD model. We consider $c_2 = -4.76$ ($M_0 = 1.25$ GeV) as the central representative case. The Lambert scale values in the corresponding cases are for the QCD coupling parameter value $\alpha_s^{(\overline{MS})}(M_Z^2) = 0.1184$.}
\end{table}

($\approx 6.45$ GeV). At $|Q^2| > (2m_\nu)^2$ (where $N_\ell \geq 4$) it is replaced by the underlying pQCD with the coupling $a_{pt}(Q^2)$, Eq. (16). The Lambert scale $\Lambda^2 = \Lambda_{|\lambda|}^2 (\sim 0.1$ GeV), which is the only on-dimensional parameter of the model, is determined by the world average value $a_{pt}(M_Z^2, \overline{MS}) = (0.1184 \pm 0.0007)/\pi$, [39]. For example, when $c_2 = -4.76$, we obtain $\Lambda \approx (0.260 \pm 0.008)$ GeV. On the other hand, the five mentioned dimensionless parameters $s_j$ and $f_j^2$ are fixed, independently of the value of $\Lambda$, by the condition Eq. (12) with $n = 5$ (these are four conditions)

$$A_1^{(\nu)}(Q^2) - a_{pt}(Q^2) \sim \left(\frac{\Lambda^2}{Q^2}\right)^5, \quad (|Q^2| > \Lambda^2), \quad (20)$$

and by the condition that the mentioned central experimental value of the strangeless $(V + A)$ $\tau$-decay ratio $r_\tau$ be reproduced by the model, namely $r_\tau = 203$. More specifically, the (four) conditions Eq. (20) determine the four parameters $s_j$ and $f_j^2$ ($j = 1, 2$) as a function of $s_0$; the value of $s_0$ ($= M_0^2/\Lambda^2$) is then determined (if $\Lambda$ is already fixed) by the condition $r_\tau = 203$. The (scheme) parameter $c_2$ remains the only free parameter of the model.

In Table I we present the results of the model for three representative values of the parameter $c_2$. The Lambert scale parameter was fixed by using the central value $0.1184/\pi$ of the world average $a_{pt}(M_Z^2, \overline{MS}) = (0.1184 \pm 0.0007)/\pi$, [40]. It turns out that increasing $c_2$ increases the pQCD-onset scale $M_0 = (s_0/\Lambda^2)$, but decreases the coupling $A_1(0)$ at $Q^2 = 0$. For phenomenological reasons, we prefer to have the scale $M_0$ ($\sim 1$ GeV) below the $\tau$ lepton mass $m_\tau$, e.g., $1$ GeV $\leq M_0 \leq 1.5$ GeV; and the value of $A_1(0)$ below unity to avoid instabilities in the infrared. These two restrictions give us the range of the free parameter $c_2$ between $-5.73$ and $-2.10$, as seen in Table I. Our central preferred value for $c_2$ is $c_2 = -4.76$, for which the pQCD-onset scale becomes $M_0 = 1.25$ GeV.

The (scheme) parameter $c_2$ in Table I was varied at fixed value $a_{pt}(M_Z^2, \overline{MS}) = 0.1184/\pi$ so that the relations [20] and $r_\tau = 203$ were fulfilled. On the other hand, if we vary the coupling parameter within the world average interval, $a_{pt}(M_Z^2, \overline{MS}) = (0.1184 \pm 0.0007)/\pi$, and keep the dimensionless parameters of the model fixed (Table I), the line with $c_2 = -4.76$, the relation [20] remains fulfilled and only the Lambert scale $\Lambda$ varies, this resulting in $r_\tau = 203 \pm 0.006$. This is acceptably compatible with the measured values $(r_\tau)_{\text{exp}} = 0.203 \pm 0.004$ [60, 61].

For further details on the 2\$\delta$anQCD model we refer to Ref. [34].

The higher order couplings $A_\nu \equiv (a_{pt}^{(\nu)})_{\text{an}}$ in this model are then obtained according to the construction for general anQCD models, explained in Refs. [22, 23] for integer $\nu$, and in Ref. [46] for general (noninteger) $\nu$ and for the couplings $A_{\nu,k} \equiv (a_{pt}^{(\nu)} \ln^k a_{pt})_{\text{an}}$. The details are given here in Appendix A.

The analytization of expansions now consists simply in the replacements

\begin{equation}
(a_{pt}^{(\nu)}(\mu^2))_\text{an} = A_\nu(\mu^2), \quad (21a)
\end{equation}

\begin{equation}
(a_{pt}(\mu^2))_\text{an} = A_{\nu,k}(\mu^2). \quad (21b)
\end{equation}

In the special case of APT, i.e., $A_1^{\text{APT}}(Q^2)$ of Ref. [11], the analytization procedure of Appendix A is, in principle, equivalent to that of Eqs. (2)-(3), as argued in Refs. [23, 46]. The (small) differences between the two analytizations in APT arise due to somewhat different truncations applied in the two approaches. In the FAPT procedure of Eqs. (2)-(3), applicable only in APT, usually the truncation in the loop expansion ($\leq a_{pt}^{(\pm 1)}$) is applied to the running coupling $a_{pt}(\mu^2)$, which is then reflected in the spectral functions $\text{Im} a_{pt}^{(\nu)}(-\sigma - i\epsilon)$ and $\text{Im}[a_{pt}^{(\nu)}(-\sigma - i\epsilon) \ln^k a_{pt}(-\sigma - i\epsilon)]$ in Eqs. (2)-(3). In the general approach, Eqs. (A7)-(A10) of Appendix A which can be applied also to the APT analytic model of $A_1(Q^2)_{\text{APT}}$ of Ref. [11], the same kind of truncation for $a_{pt}(\mu^2)$ can be applied in $\rho_1^{(\text{pt})}(\sigma) = \text{Im} a_{pt}(Q^2 = -\sigma - i\epsilon)$, 

\footnote{In Ref. [33] we included the case $c_2 = -7.15$, for which $M_0 = 1.0$ GeV. However, in that case, $A_1(0) = 2.29$, and this indicates that the model is unstable in the infrared at such $c_2$ values.}
in the integral [A7]; in addition, the corresponding loop-truncation in the summations [A9] and [A10] is applied – usually \( m \leq \ell - \nu \).

Figure 2(b) shows that the logarithmic derivatives \( \tilde{A}_2(\mu^2) \) of the \( 2\delta \)anQCD model are almost indistinguishable from each other at \( \mu^2 > 1 \) GeV\(^2\), this being the consequence of the construction of the \( 2\delta \)anQCD model: \( A_1(\mu^2) - a_{pt,2}(\mu^2) \sim (\Lambda^2/\mu^2)^5 \) for \( |\mu^2| > \Lambda^2 \). Namely, application of \( d/d\ln \mu^2 \) to this relation implies \( \tilde{A}_2(\mu^2) - \tilde{a}_{pt,2}(\mu^2) \sim (\Lambda^2/\mu^2)^5 \). On the other hand, Fig. 2(a) shows that the difference between \( A_2(\mu^2) \) and \( a_{pt}(\mu^2) \) is significant even up to \( \mu^2 \approx 5 \) GeV\(^2\), this being the consequence of the aforementioned truncation at \( \tilde{A}_5 \) in the construction of \( A_2 \) (Appendix A).
III. PERTURBATION EXPANSION FOR HEAVY $q\bar{q}$ GROUND STATE ENERGY

A. General formulas

The analysis of nonrelativistic potential is the starting point for the determination of the ground state energy of $q\bar{q}$ and thus of the mass of such systems. The main input in these calculations is the mass $\overline{m}_q(m_q^2)$ (here denoted simply as $\overline{m}_q$), also called $\overline{M}_S$ quark mass. The masses of the heavy quarkonia $\bar{q}q$ [Υ(1S) when $q = b$, $J/\psi(1S)$ when $q = c$] are well measured, and this allows us to extract the corresponding mass $\overline{m}_q$. By evaluating an observable, such as the quark-antiquark binding energy here, within anQCD models, at least part of the (chirality-conserving) nonperturbative effects get included in the leading-twist term via the analytization, such as Eqs. (2)-(3) in (F)APT, and (21) in general analytic QCD models.

The coefficients in the (leading-twist) perturbation expansion of the ground state binding energy $E_{qq}$ (i.e., with: $n = 1$ and $\ell = 0$) of heavy quarkonium $q\bar{q}$ in powers of $a_{pt}$ were obtained up to all terms $\mathcal{O}(a_{pt}^5)$ in Ref. [52], the terms $\mathcal{O}(a_{pt}^5)$ in $a_{pt}$ in Ref. [63], and all terms up to $\mathcal{O}(a_{pt}^5)$ (including logarithmic) are given in Ref. [7]. The last term ($\sim a_{pt}^5$) is now completely known since the parameter $a_3$ from the static potential is now known, Refs. [5, 6]. The general structure of the (leading-twist term of the) ground state binding energy in pQCD is

$$E_{qq}^{(pt)} = -\frac{4}{9} m_q \pi^2 a_{pt}^2 (\mu^2)^2 \left\{ 1 + a_{pt}(\mu^2) \left[ K_{1,0} + K_{1,1} L_{pt}(\mu^2) \right] + a_{pt}^2(\mu^2) \left[ K_{2,0} + K_{2,1} L_{pt}(\mu^2) + K_{2,2} L_{pt}^2(\mu^2) \right] ight\} \mu^2,$$

(22)

where

$$L_{pt}(\mu^2; m_q^2) = \frac{1}{2} \ln \left( \frac{\mu^2}{(4\pi/3) a_{pt}^2 (\mu^2)} \right),$$

(23)

$\mu^2$ is the (square of the) renormalization scale, $m_q$ is the pole mass of the quark, and the coefficients $K_{j,k}$ can be obtained by combining the results of the mentioned literature; cf. Appendix B. The typical scale of the process is a soft reference scale $Q^2$ ($\equiv -q^2$), which is a typical quark-antiquark momentum transfer inside the quarkonium $(Q_s^2 \sim m_q^2 \alpha_s^2)$ and can be fixed by convention. The soft renormalization scale $\mu^2 \equiv \mu_s^2$ can then be varied around $Q_s^2$.

$$\mu^2 \equiv \mu_s^2 = \kappa Q_s^2 \quad (\kappa \sim 1; Q_s^2 \sim m_q^2 \alpha_s^2).$$

(24)

The quarkonium mass is then

$$M_{qq} = 2 m_q + E_{qq}(m_q).$$

(25)

In principle, the input quantity here could be the quark pole mass $m_q$. However, this mass $m_q$, in contrast to the mass $\overline{m}_q$, suffers from the strong infrared renormalon ambiguity (at Borel parameter value $b = 1/2$, $\Rightarrow \delta m_q \sim \Lambda_{QCD}$). This ambiguity must cancel in the physical sum [Eq. (25)].

It is more convenient to use as input a renormalon ambiguity-free input mass, such as $\overline{m}_q$, and we will do this.

In the case of the bottom quark, before we relate the pole mass $m_b$ with the mass $\overline{m}_b$, at renormalization energies $\mu = \overline{m}_b$ where $N_f = 4$ (and where the charm quark mass is considered zero, i.e., decoupled), the effects $\delta m_b$ of the nonzero mass $m_c \neq 0$ have to be subtracted, and they are [64]

$$\langle \delta m_b \rangle_{m_c} = \langle \delta m_b \rangle_{m_c}^{(1)} \approx \delta m_b \approx 0.025 \pm 0.005 \text{ GeV}.$$

(26)

These effects were calculated in Ref. [64] in pQCD, at the hard renormalization scale $\mu^2 = \overline{m}_b^2$. We checked that they do not get significantly modified in APT and in the $2\delta m\overline{n}QCD$ model.

The pole mass $m_q$ and the mass $\overline{m}_q$ are then related via the relation

$$m_q - \delta m_q = \frac{m_q}{\overline{m}_q} = 1 + \frac{4}{3} \left( a_{pt}(\overline{m}_q^2) + r_1 a_{pt}^2(\overline{m}_q^2) + r_2 a_{pt}^3(\overline{m}_q^2) + r_3 a_{pt}^4(\overline{m}_q^2) \right) + \mathcal{O}(a_{pt}^5),$$

(27)

where $\delta m_q$ is zero when $q = c$, and is given by Eq. (26) when $q = b$

$$\delta m_q \equiv \left\{ \begin{array}{ll} \langle \delta m_b \rangle_{m_c} \quad (q = b) \\ 0 \quad (q = c) \end{array} \right\}. $$

(28)
The coefficient $R_0 = 4/3$ was obtained in Ref. [65]. Also the coefficients \( r_1(\bar{m}_q^2) \), and \( r_2(\bar{m}_q^2) \) are known (Refs. [66, 67, 69], respectively) they are given in Eqs. (C1) in Appendix C, and \( N_f \) in these coefficients is the number of flavors of quarks lighter than \( q \). Specifically, the values are: \( r_1 = 7.739 \) and \( r_2 = 87.224 \) for \( N_f = 3 \); and \( r_1 = 6.958 \) and \( r_2 = 70.659 \) for \( N_f = 4 \). On the other hand, in Appendix C we estimate the values of \( r_3 \) to a reasonably high level of precision (with less than 4% uncertainty) by a method which uses the structure of the leading infrared renormalon (at \( b = 1/2 \)) of the quantity \( m_q/\bar{m}_q \): \( r_3(N_f = 3) = 1339.4 \), \( r_3(N_f = 4) = 987.3 \).

While the relation (27) is written here at the “hard” renormalization scale \( \mu^2 = \bar{m}_q^2 \), it is straightforward to reexpress the sum on the right-hand side of Eq. (27) at a different, lower, scale \( \mu^2 \). In Appendix C this reexpression is presented explicitly, under the assumption that during the lowering of the scale, \( \bar{m}_q^2 \rightarrow \mu^2 \), we do not cross the quark threshold. The goal is to express in the perturbation expansion of the binding energy (22), where the renormalization scale is soft, the pole mass \( m_q \) via the mass \( \bar{m}_q \), and for this we need the relation (27) at the soft renormalization scale. It turns out that for the \( b\bar{b} \) system the hard scale is \( \bar{m}_b \approx 4 \text{ GeV} \), i.e., the scale where \( N_f = 4 \); and the soft scale, Eq. (24), is \( \mu_s \approx 2 \text{ GeV} \), i.e., the scale where it is more reasonable to expect \( N_f = 3 \). In this case, we take into account also the (three-loop) quark threshold transition \( N_f = 4 \rightarrow 3 \) at \( \mu^2 = (2m_s)^2 \), Ref. [70]. We thus obtain the relation (27) reexpressed at the soft scale \( \mu_s^2 \) of Eq. (24)

\[
\delta m_q(\bar{m}_q^2; \mu_s^2) = \delta m_q + \bar{m}_q \left\{ 1 + \frac{4}{3} a_{pt}(\mu_s^2) \left[ 1 + a_{pt}(\mu_s^2)r_1(\mu_s^2) + a_{pt}(\mu_s^2)r_2(\mu_s^2) + a_{pt}(\mu_s^2)r_3(\mu_s^2) \right] + \mathcal{O}(a_{pt}^3) \right\} .
\]  

(29)

Further, the renormalization scheme can also be varied in this relation and in the relations (22, 23), i.e., the changes of the scheme parameters \( c_j = \beta_j/\beta_0 \) for \( j = 2, 3 \) from the usual \( \overline{\text{MS}} \) scheme to other schemes affect correspondingly the values of the coupling \( a_{pt}(\mu_s^2) \) and of the coefficients. We recall that in (F)APR the chosen scheme here is \( c_2 = c_3 = \cdots = 0 \); in the 2\( \delta \)anQCD model and in Lambert pQCD, the scheme is \( c_2 = -4.76_{-0.66}^{+2.66} \) and \( c_j = c_2^{-1}/c_j^{1/2} \) for \( j \geq 3 \). The relationship between \( a_{pt} \)'s at two different scales and in two different renormalization schemes is summarized in Appendix D where we also summarize the (three-loop) connection of \( a_{pt} \)'s across the quark threshold. After performing all these transformations, we can rewrite the original expansion (22) for \( E_{qq} \) in terms of the \( \bar{m}_q \equiv \bar{m}_q(\bar{m}_q^2) \) mass, with the coupling \( a_{pt} \), at any soft renormalization scale \( \mu_s \) and in any chosen renormalization scheme (\( c_2, c_3, \ldots \))

\[
E_{qq}(Q_s^2; \bar{m}_q^2; N_f = 3) = -\frac{4}{9} \bar{m}_q + \delta m_q + a_{pt}(\mu_s^2) \left\{ 1 + a_{pt}(\mu_s^2) \left[ K_{1,0} + K_{1,1} \mathcal{L}_{pt}(\mu_s^2) \right] \right\}
+ a_{pt}^2(\mu_s^2) \left\{ K_{2,0} + K_{2,1} \mathcal{L}_{pt}(\mu_s^2) + K_{2,2} \mathcal{L}_{pt}^2(\mu_s^2) \right\}
+ \frac{1}{2} a_{pt}^3(\mu_s^2) \left\{ K_{3,0,0} + K_{3,0,1} \ln a_{pt}(\mu_s^2) + K_{3,1} \mathcal{L}_{pt}(\mu_s^2) + K_{3,2} \mathcal{L}_{pt}^2(\mu_s^2) + K_{3,3} \mathcal{L}_{pt}^3(\mu_s^2) \right\} + \mathcal{O}(a_{pt}^4) \right\} ,
\]

(30)

where \( \mu_s^2 = \kappa Q_s^2 \) (\( \kappa \sim 1 \)) being the soft renormalization scale parameter, and the logarithm contains now \( \bar{m}_q \) mass

\[
\mathcal{L}_{pt}(\mu_s^2; \bar{m}_q^2) = \frac{1}{2} \ln \left( \frac{\mu_s^2}{(4\pi/3)(\bar{m}_q + \delta m_q))^2 a_{pt}^2(\mu_s^2)} \right) .
\]

(31)

We note that the new (renormalon-ambiguity-free) mass which appears naturally in this expansion is not exactly the mass \( \bar{m}_q \), but rather

\[
\bar{m}_q \equiv m_q + \delta m_q = \begin{cases} m_b + (\delta m_b)_{m_c} & (q = b) \\ m_c + (\delta m_c)_{m_b} & (q = c) \end{cases}
\]

(32)

where \( (\delta m_q)_{m_c} \) is given by Eq. (26) when \( q = b \).

The mentioned soft “process scale” \( Q_s^2 \) (\( \sim m_q^2 \alpha_s^2 \)) can be regarded, at least formally, to be a variable complex scale. Therefore, the binding energy \( E_{qq}(Q_s^2; \bar{m}_q^2) \) is, formally, a spacelike observable analytic in \( Q_s^2 \); and the dependence on the renormalization scale parameter \( \kappa \) disappears when the number of terms in the expansion is infinite. The

12 Usually, the quark thresholds are taken at \( 2m_q \). In the case of \( N_f = 4 \rightarrow 3 \) transition, this is about 2.5 GeV, above the soft scale of the \( b\bar{b} \) system.
analytization of $E_{qq}^{(pt)}(Q_s^2; m_q^2)$ of Eq. (30), according to Eqs. (21) [or, in (F)APT: Eqs. (22-3)], then leads to

$$E_{qq}^{(an)}(Q_s^2; m_q^2) = -\frac{4}{9} \bar{m}_q \pi^2 \{ A_2(\kappa Q_s^2) + [K_{1,0} A_3(\kappa Q_s^2) + K_{1,1} B_{3,1}(\kappa Q_s^2)] + [K_{2,0} A_4(\kappa Q_s^2) + K_{2,1} B_{4,1}(\kappa Q_s^2) + K_{2,2} B_{4,2}(\kappa Q_s^2)] + [K_{3,0,0} A_5(\kappa Q_s^2) + K_{3,0,1} A_5(\kappa Q_s^2) + K_{3,1} B_{5,1}(\kappa Q_s^2) + K_{3,2} B_{5,2}(\kappa Q_s^2) + K_{3,3} B_{5,3}(\kappa Q_s^2)] + O(A_{6,4}) \}, \quad (33)$$

where we use, for simplicity, the notation of Eq. (A9) with Eq. (A5) for $A_\nu$’s ($\nu = k$ integer now) [in (F)APT: Eq. (2)], and denote by $B_{n+2,j}$ the following:

$$B_{n+2,j}(\kappa Q_s^2) = \left( a_{pt}^{n+2}(\kappa Q_s^2) \right) \ln \left( \frac{\kappa Q_s^2}{(4\pi/3)m_q^2a_{pt}^2(\kappa Q_s^2)} \right) \quad \text{where} \quad \tilde{m}_q = \delta m_q + m_q \left\{ 1 + \frac{4}{3} \right\} = 0 \right\} + O(A_5) \} , \quad (34)$$

where $\tilde{m}_q$ is defined in Eq. (32). This type of condition, in analytic QCD, would correspond to fixing the soft reference scale $Q_s^2$ by requiring $B_{n+1,j}(Q_s^2) = 0$, for various $n$’s and $j = 1, \ldots, n$. This fixing is not unique since it depends on $n$ and $j$. Our convention will be that the leading logarithmic term in Eq. (33) is zero at such scale

$$B_{3,1}(Q_s^2) = 0 . \quad (37)$$

It will turn out that this condition has a solution in the case of $b\bar{b}$ ($\Upsilon(1S)$) in the 2$\delta$anQCD model, but not in $J/\psi(1S)$ in that model, and not in any case of the (F)APT model. In such respective cases, we will use simply the following simpler analogs of the pQCD condition (36).

$$Q_s^{2,((F)\text{APT})} = (4\pi/3)^2 \tilde{m}_q^2 A_2((F)\text{APT})(Q_s^{2,((F)\text{APT})}) \quad (39)$$

These measures of the typical momentum scale of the (nonrelativistic) quark inside the quarkonium are rather low, $\approx 2 \text{ GeV} in \Upsilon(1S)$, and $\lesssim 1 \text{ GeV} in J/\psi(1S)$. In pQCD such scales are problematic, because they are not far away from the unphysical (Landau) singularities of $a_{pt}(Q_s^2)$; in analytic QCD models, no such problems appear in principle.

### B. Separation of the soft and ultrasoft contributions

The pole mass $m_q$ and the static potential $V(r)$ both contain the leading infrared renormalon ($b = 1/2$) singularities, and cancellation of these singularities takes place in the sum $2m_q + V(r)$ [71,73]. As a consequence, this cancellation must take place also in the quarkonium mass $2m_q + E_{qq}^{(pt)}$ [64,74,78], more specifically, in the sum $2m_q + E_{qq}(s)$ where $E_{qq}(s) = (1|V(r)|1)$ [~$V(r)$] is the soft part of the binding energy $E_{qq}$, and $|1|$ denotes the (ground) state of the quarkonium. The typical soft distance $r_s$ in the quarkonium is $\sim 1/\sqrt{q^2}$, where $a = a_{pt}$ or $A_1$. Since
V(r_s) \propto 1/r_s, we have $E_{q\bar{q}}(s)/m_q \sim V(r_s)/m_q \propto 1/(r_s m_q) \sim (\pi a)$. This leads to the so called “power mismatch” in the renormalon cancellation in the pQCD expansion of the sum $(2m_q + E_{q\bar{q}}(s))/m_q$ [see also: 79]: the terms $\sim a^n$ in $2m_q/m_q$ tend to cancel numerically the terms $\sim a^{n+1}$ in $E_{q\bar{q}}(s)/m_q$. Therefore, since the binding energy $E_{q\bar{q}}$ is now known up to $\sim a_3^0$, it is very convenient to have the relation $m_q/m_q$ up to $\sim a_4^0$, i.e., to have a good estimate for the coefficient $r_3$ and use it, so that the effects of renormalon cancellation in $2m_q + E_{q\bar{q}}(s)$ can be seen numerically more clearly. This was the main reason for performing the analysis in Appendix C, resulting in estimates of $r_3$, Eq. (C13). This cancellation, term by term, should be numerically more precise (at sufficiently high orders) if the renormalization scales $\mu_s$ used in $m_q/m_q$ and in $E_{q\bar{q}}(s)/m_q$ [Eqs. (29) and (30)] are taken to be equal. This renormalon cancellation will be our guiding principle for the separation of the soft (s) and the ultrasoft (us) part in the binding energy

$$E_{q\bar{q}} = E_{q\bar{q}}(s) + E_{q\bar{q}}(us).$$

Typical us scales are $\mu_{us} \sim m_q a_2^0$, and the us part of the binding energy is $\sim m_q a^5 \ln a$. We can parametrize the s-us separation by a dimensionless parameter $k_{s/us}$ such that the s-us factorization scale $\mu_f$ is written as

$$\mu_f = k_{s/us} m_q a_2^0 (Q_s)^{3/2} \left[ \approx k_{s/us} (Q_s Q_{us})^{1/2} \right],$$

where $Q_{us} \sim m_q a_2^0$ is a (chosen) us reference scale. It is expected that usually $k_{s/us} \sim 1$, but it does not have to be so always. The us part can be rewritten, in terms of $k_{s/us}$ as (cf. Ref. 78)

$$E_{q\bar{q}}^{(pt)}(us) = -\frac{4}{9} m_q \pi^2 \left[ K_{3,0,0}(us) a_5^{(pt)}(\mu_f^{us}) + K_{3,0,1}(us) a_5^{(pt)}(\mu_f^{us}) \ln a_{pt}(\mu_f^{us}) + O(a_{pt}^3) \right],$$

and in analytic QCD correspondingly

$$E_{q\bar{q}}^{(an)}(us) = -\frac{4}{9} m_q \pi^2 \left[ K_{3,0,0}(us) A_5(\mu_f^{us}) + K_{3,0,1}(us) A_{5,1}(\mu_f^{us}) + O(A_6) \right],$$

where $\mu_{us} = k_{s/us} Q_{us}$ is a us renormalization scale ($k_{s/us} \sim 1$), and the two us coefficients are

$$K_{3,0,1}(us) = 7.098 \pi^3, \quad K_{3,0,0}(us) = \left[ 27.512 + 7.098 \ln \pi - 14.196 \ln(k_{s/us}) \right] \pi^3.$$  

The expansion of the soft (s) part $E_{q\bar{q}}(s)$ of the binding energy is then, according to Eq. (40), the same as the expansions (30) and (33), with the exception of the replacements of two coefficients $K_{3,0,0}$ and $K_{3,0,1}$

$$E_{q\bar{q}}^{(pt,an)}(s) = E_{q\bar{q}}^{(pt,an)}(k_{3,0,0} \rightarrow K_{3,0,0} - K_{3,0,0}(us); K_{3,0,1} \rightarrow K_{3,0,1} - K_{3,0,1}(us)).$$

The s-us factorization, i.e., the parameter $k_{s/us}$, will then be determined, in each model, by requiring that the leading infrared renormalon cancellation in $2m_q + E_{q\bar{q}}(s)$ be exact at the last available order, i.e., that the $O(a^n)$ term in $2m_q(Q_s^2/m_q^2)$ and the term $O(a^5)$14 in $E_{q\bar{q}}(s; Q_s^2/m_q^2)$ cancel exactly.

The us part of the quarkonium mass, $E_{q\bar{q}}(us; Q_s^2/m_q^2)$, will be evaluated in each case according to a procedure which takes into account those problems of low-scale evaluations which appear in the considered model (2\textsubscript{\textsc{fanQCD}}, pQCD, (F)AP). We recall that the binding energy $E_{q\bar{q}}(s)$ is a Euclidean quantity because it depends on spacelike quark-antiquark momentum transfer $q$ ($q^2 = -\bar{q}^2 = -Q^2 < 0$). Analytization of such quantities must follow the procedure 21. On the other hand, the quark pole mass $m_q$ is a Minkowskian quantity because it depends on the timelike pole momentum ($q^2 = -\bar{q}^2 = m_q^2 > 0$). We note that our analytization procedure for the quark pole mass is again the procedure $a_n^{pt}(m_q^2) \rightarrow A_n(m_q^2)$ in the relation 27 [and then reexpressing $A_n(m_q^2)$ via $A_k(\mu_f^2)$'s at a lower soft scale $\mu_f^2$, for renormalon cancellation]. This procedure, for the Minkowskian quantities, is analogous to the fixed order perturbation theory (FOPT) in pQCD, Ref. 80, where the couplings in the corresponding contour integral, on the contour $Q^2 = m_q^2 \exp(i\phi)$, are Taylor-expanded around the spacelike point $Q^2 = m_q^2 > 0$. As a result, the kinematic $\pi^2$-terms appear in the expansion coefficients $r_j$.

13 The coefficients $K_{3,0,0}(us)$ and $K_{3,0,1}(us)$, representing the leading part of the (quasi)observable $E_{q\bar{q}}(us)$, are renormalization scale ($\mu_{us}$) and scheme independent.

14 The latter term includes all $O(a^n \ln k a)$ terms ($k = 0, 1, 2, 3$).
Another analytization of the pole mass expansion would involve contour integration of the corresponding Euclidean quantity with (exact) RGE-running couplings along the contour, cf. Ref. [81]. This procedure is analogous to the Contour Improved Perturbation Theory (CIPT) in pQCD; in such a case, the aforementioned $\pi^2$ terms are effectively resummed, Refs. [82, 83]. We decided not to pursue this CIPT type of analytization, because it is technically more demanding due to the additional running of the mass factor $\bar{m}_q(\mu^2)$; and because in this approach the renormalon cancellation mechanism, due to the mentioned resummations, probably changes its practical form. This problem remains to be addressed in the future.

IV. NUMERICAL RESULTS

A. Bottom mass extraction

In this section, we extract from the mass of $b\bar{b}$ quarkonium the mass $\bar{m}_b \equiv \bar{m}_b(\bar{m}_b^2)$ in (F)APT, 2δanQCD model, and in pQCD in two renormalization schemes (\MSbar and in the Lambert scheme of 2δanQCD). For this, we use the relation between $\bar{m}_b$ and the well-measured mass of the $b\bar{b}$ quarkonium $\Upsilon(1S)$ [49]

$$2m_b(\bar{m}_b^2; \mu_s^2) + E_{bb}(s; Q_s^2; \bar{m}_b^2; \mu_s^2, N_f = 3) + E_{bb}(us; Q_{us}^2; \bar{m}_b^2; \mu_s^2) = M_{\Upsilon(1S)}^{(exp)}(= 9.460 \text{ GeV}) \, .$$

(46)

The dependence on the (soft) renormalization scale $\mu_s^2 = \kappa_s Q_s^2$ in the pole mass $m_b$ and in the soft binding energy $E_{bb}(s)$ occurs due to the truncation of the series by the for these two quantities. For the same reason, the ultrasoft binding energy $E_{bb}(us)$ has strong dependence on the ultrasoft renormalization scale $\mu_s^2(= \kappa_s Q_{us}^2)$ due to the drastic truncation of this quantity at its leading order ($\sim a^3 \ln a$). As mentioned in the previous Section, the separation of the $s$ and $us$ parts of the binding energy will be performed here by determining the $s$-$us$ separation parameter $k_{s/us}$, Eqs. [10]-[15], by the requirement of cancellation of the leading renormalon in $2m_b + E_{bb}(s)$.

In contrast to the other three models, (F)APT gives a very small central value for the $s$-$us$ separation parameter $k_{s/us} \approx 6 \times 10^{-10}$. This reflects the difficulty in the (F)APT scenario to exactly enforce the leading renormalon cancellation of the $\sim A_1$ term of $2m_b$ with the corresponding $\sim A_5$ term of $E_{bb}(s)$. If, on the other hand, we impose in (F)APT the condition $k_{s/us} \sim 1$, more specifically the central value $k_{s/us} = 1$ and variation in the interval $(0.1,1.0)$, the results change somewhat, the central extracted value of $\bar{m}_b$ increases by about 0.050 GeV, and the absolute values of the $us$ part of the binding energy and of various other uncertainties of $\bar{m}_b$ get reduced. We will consider in (F)APT only the natural range $\sim 1$ of the $s$-$us$ separation parameter, $k_{s/us} = 1.0^{-0.9}$, rather than the exceedingly small values of $k_{s/us}$ required by the exact renormalon cancellation. In the other three models (2δanQCD, and in Lambert and \MSbar pQCD), the renormalon cancellation is imposed without any problems, resulting in the values of $k_{s/us}$ within the interval between $10^{-1}$ and $10^1$.

In the previous section we mentioned that we take $N_f = 3$ for the number of active flavors in the binding energy, i.e., in this case the $m_c$ mass is considered to be infinite (decoupled). It turns out that, while the effects of the finiteness of $m_c$ cannot be neglected in the relation between $m_b$ and $\bar{m}_b$, Eqs. [26]-[27], these effects can be safely neglected in the binding energy $E_{bb}(N_f = 3)$; cf. Ref. [84] based on Refs. [60, 85, 89].

Application of the formalism described in Secs. [11A] and [11B] (with Appendix A) for the calculation of the couplings of the analytic QCD models (F)APT and 2δanQCD, and in Sec. [11] for the calculation of $2m_b$, $E_{bb}(s)$ and $E_{bb}(us)$ in terms of these couplings, then gives us the following results:

\[
\bar{m}_b(\text{(F)APT}) = \left\{ 4.155 \pm 0.002(\mu_s) + \left( \begin{array}{c} +0.005 \\ -0.004 \end{array} \right) \right\}_{(s/us)} + \left( \begin{array}{c} -0.019 \\ +0.020 \end{array} \right)_{(A)} \\
\left( \begin{array}{c} -0.004 \\ +0.002 \end{array} \right)_{(\mu_s)} = 0.005(m_c) \right\} \text{ GeV} (47a)
\]

\[
= 4.155 \pm 0.022 \text{ GeV} \, , \quad \text{with : } Q_s(\text{(F)APT}) = 1.60 \text{ GeV } , \quad k_{s/us} = 1.0 \, . (47b)
\]

\[
\bar{m}_b(2\text{δanQCD}) = \left\{ 4.353 + \left( \begin{array}{c} -0.068 \\ +0.071 \end{array} \right) \right\}_{(us)} + \left( \begin{array}{c} +0.015 \\ -0.016 \end{array} \right)_{(s/us)} \mp 0.005(m_c) \\
\left( \begin{array}{c} -0.023 \\ +0.034 \end{array} \right)_{(c_2)} + \left( \begin{array}{c} +0.017 \\ -0.025 \end{array} \right)_{(\mu_s)} \right\} \text{ GeV} (48a)
\]

\[
= 4.353 \pm 0.084 \text{ GeV} \, , \quad \text{with : } Q_s = 2.08 \text{ GeV } , \quad k_{s/us} = 0.238 \, . (48b)
\]
We will comment on the above uncertainties below. For completeness, we give here also the results of the same kind of analysis in pQCD, first in the Lambert renormalization scheme (i.e., the scheme as used in 2\delta\text{anQCD}: \(c_2 = -4.76, c_j = c_j^{\text{Lamb}}/c_j^{\text{PT}}\) for \(j \geq 3\); and in the (four-loop) MS scheme:

\[
\overline{m}_b(\text{pQCD}, \text{Lamb.}) = \left\{ 4.382 + \left( \begin{array}{c} -0.091 \\ +0.097 \end{array} \right) \right\}_{(us)} + \left( \begin{array}{c} -0.013 \\ +0.017 \end{array} \right) \right\}_{(s/\text{us})} \pm 0.010(\alpha_s) \\
+ \left( \begin{array}{c} +0.027 \\ -0.008 \end{array} \right) \right\}_{(s)} + \left( \begin{array}{c} -0.002 \\ -0.041 \end{array} \right) \right\}_{(\mu_s)} \mp 0.005(m_c) \right\} \text{GeV} \tag{49a}
\]

\[
= 4.382 \pm 0.111 \text{ GeV , with : } Q_{s,\text{PT}} = 1.73 \text{ GeV , } k_{s/\text{us}} = 0.306 . \tag{49b}
\]

\[
\overline{m}_b(\text{pQCD}, \text{MS}) = \left\{ 4.505 + \left( \begin{array}{c} -0.177 \\ +0.200 \end{array} \right) \right\}_{(us)} + \left( \begin{array}{c} -0.082 \\ +0.084 \end{array} \right) \right\}_{(s/\text{us})} + \left( \begin{array}{c} +0.031 \\ -0.027 \end{array} \right) \right\}_{(\alpha_s)} \\
+ \left( \begin{array}{c} -0.004 \\ -0.075 \end{array} \right) \right\}_{(\mu_s)} \mp 0.005(m_c) \right\} \text{GeV} \tag{50a}
\]

\[
= 4.505 \pm 0.231 \text{ GeV , with : } Q_{s,\text{PT}} = 1.87 \text{ GeV , } k_{s/\text{us}} = 0.248 . \tag{50b}
\]

The value of the s-us separation parameter \(k_{s/\text{us}}\) was determined in all cases by the aforementioned renormalon cancellation in the sum \(M_{T(1S)}(s) = 2m_b + E_{\delta\delta}(s; k_{s/\text{us}})\), except in the (F)APT case, as discussed above. Below we present these resulting sums, for the central choices of the aforementioned four results, where we combine in each parenthesis the (positive) terms \(\sim a^n\) of \(2m_b\) and the corresponding (negative) terms \(\sim a^{n+1}\) of \(E_{\delta\delta}(s)\) \((n = 0, 1, 2, 3, 4)\), in order to see more clearly the tendency of the renormalon cancellation; the us part is given separately

\[
M_{T(1S)}(s; \text{(F)APT}) = 8.361 + (1.145 - 0.152) + (0.281 - 0.174) + (0.161 - 0.154) + (0.081 - 0.093) \text{ GeV} \\
= 8.361 + 0.993 + 0.107 + 0.060 - 0.013 \text{ GeV (} = 9.454 \text{ GeV) ,} \tag{51a}
\]

\[
E_{\delta\delta}(us; \text{(F)APT}) = 0.006 \mp 0.003 \text{ GeV , (} \overline{m}_b = 4.155 \text{ GeV, } k_{s/\text{us}} = 1.0) ; \tag{51b}
\]

\[
M_{T(1S)}(s; 2\delta\text{anQCD}) = 8.756 + (0.999 - 0.131) + (0.373 - 0.222) + (0.233 - 0.193) + (0.568 - 0.568) \text{ GeV} \\
= 8.756 + 0.868 + 0.151 + 0.040 + 0.000 \text{ GeV (} = 9.815 \text{ GeV) ,} \tag{52a}
\]

\[
E_{\delta\delta}(us; 2\delta\text{anQCD}) = -0.355 \pm 0.151 \text{ GeV , (} \overline{m}_b = 4.355 \text{ GeV, } k_{s/\text{us}} = 0.238) ; \tag{52b}
\]

\[
M_{T(1S)}(s; \text{pQCD}, \text{Lamb.}) = 8.814 + (1.095 - 0.170) + (0.327 - 0.220) + (0.346 - 0.376) + (0.413 - 0.413) \text{ GeV} \\
= 8.814 + 0.925 + 0.107 - 0.031 + 0.000 \text{ GeV (} = 9.816 \text{ GeV) ,} \tag{53a}
\]

\[
E_{\delta\delta}(us; \text{pQCD}, \text{Lamb.}) = -0.355 \pm 0.201 \text{ GeV , (} \overline{m}_b = 4.382 \text{ GeV, } k_{s/\text{us}} = 0.306) ; \tag{53b}
\]

\[
M_{T(1S)}(s; \text{pQCD}, \text{MS}) = 9.060 + (1.183 - 0.193) + (0.399 - 0.263) + (0.330 - 0.439) + (0.475 - 0.475) \text{ GeV} \\
= 9.060 + 0.991 + 0.136 - 0.109 + 0.000 \text{ GeV (} = 10.078 \text{ GeV) ,} \tag{54a}
\]

\[
E_{\delta\delta}(us; \text{pQCD}, \text{MS}) = -0.617 \pm 0.394 \text{ GeV , (} \overline{m}_b = 4.505 \text{ GeV, } k_{s/\text{us}} = 0.248) ; \tag{54b}
\]

We can see from Eqs. (51a)-(54a) explicitly that for the chosen corresponding central values of the parameter \(k_{s/\text{us}}\) the renormalon cancellation is exact in the last term [the fifth term, named \(t_5(s)\)] in the sum for the soft mass \(M_{T(1S)}(s)\), except in the case of (F)APT where \(k_{s/\text{us}} = 1.0\) was chosen and the cancellation in \(t_5(s)\) is approximate.

The extracted values of \(\overline{m}_b\), Eqs. (51)-(54), have a strong uncertainty coming from the ultrasoft (us) regime and from the related s-us separation. The origin of this uncertainty lies in the strong dependence of the us binding energy \(E_{\delta\delta}(us; \mu^2_{us})\) on the us renormalization scale \(\mu_{us}\) and on the s-us separation parameter \(k_{s/\text{us}}\), cf. Eqs. (41)-(44). The behavior of the us binding energy \(E_{\delta\delta}(us; \mu^2_{us})\) in the three models (2\delta\text{anQCD}, and pQCD in the two schemes), as a function of the us renormalization scales \(\mu_{us}\) in the low-momentum regime, is presented in Fig. 3(a), and in the case of (F)APT in Fig. 3(b). In the 2\delta\text{anQCD} model and in pQCD, we do not consider the scales \(\mu_{us}\) below \(\mu_{us}^{\text{min}} = 1.1\)
We recall that in the $2 \delta \text{anQCD}$ model the part of the binding energy $E_{bb}(us)$, for the central input values of the $2 \delta \text{anQCD}$ model, however, is fixed according to Eq. (39) and gives, for the central values of the input parameters, the value $E_{bb}(us; 1.15 \text{ GeV})$ when Landau singularities (poles and cuts) appear at scales $\mu_{us} < 1.1 \text{ GeV}$ and $1.2 \text{ GeV}$ in the $2 \delta \text{anQCD}$ model and in pQCD. Therefore, we estimate the $us$ binding energy in the following way [we use the notation $E_{bb}(us; \mu_{us}^2)$]:

$$E_{bb}(us; 2 \delta \text{anQCD}) = \frac{1}{2} [E_{bb}(us; \mu_{us}^2) - (E_{bb}(us)_{\min})^2] + \frac{1}{2} [E_{bb}(us; \mu_{us}^2) - (E_{bb}(us)_{\min})^2],$$

where the soft reference scale $Q_s$ was determined by the condition (37), and gave for the central values of the input parameters, the soft reference scale value $Q_s = 2.08 \text{ GeV}$.

In the two pQCD approaches, $E_{bb}(us)$ decreases monotonously when $\mu_{us}$ decreases below the soft reference scale $Q_{s,pt}$ of Eq. (30). For pQCD in the Lambert scheme ($c_2 = -4.76$), with central values of the input parameters, the soft reference scale turns out to be $Q_{s,pt} \approx 1.73 \text{ GeV}$, and the $us$ binding energy at $(\mu_{us})_{\min} = 1.1 \text{ GeV}$ reaches the value of $-0.56 \text{ GeV}$. In the $\overline{\text{MS}}$ scheme, however, $E_{bb}(us; 1.13 \text{ GeV})^2 \approx -1.5 \text{ GeV}$, which is exceedingly low and indicates failure of the method already at such scales, due to vicinity of Landau singularities of the running coupling. Therefore, in $\overline{\text{MS}}$ we take as the minimal acceptable scale $(\mu_{us})_{\min} = 1.2 \text{ GeV}$, where $E_{bb}(us; 1.2 \text{ GeV})^2 \approx -1.0 \text{ GeV}$ and $Q_{s,pt} \approx 1.87 \text{ GeV}$ when the central values of the input parameters are used. Thus, in pQCD we estimate the $us$ binding energy as

$$E_{bb}(us) = \frac{1}{2} [E_{bb}(us; \mu_{us}^2) - (E_{bb}(us)_{\min})^2] + \frac{1}{2} [E_{bb}(us; \mu_{us}^2) - (E_{bb}(us)_{\min})^2],$$

with $(\mu_{us})_{\min} = 1.1 \text{ GeV}$ and $2 \text{ GeV}$ in the Lambert and $\overline{\text{MS}}$ schemes, respectively.

In the (F)APT case, on the other hand, $Q_s$ is fixed according to Eq. (39) and gives, for the central input parameter values, the value $Q_s((\text{F})\text{APT}) = 1.60 \text{ GeV}$. In (F)APT no practical problems appear at scales $\mu_{us} < 1.1 \text{ GeV}$, $E_{bb}(us, (\text{F})\text{APT})$ reaches a moderate maximum value of $0.009 \text{ GeV}$ at $\mu_{us} \approx 0.7 \text{ GeV}$ for the chosen central value

\[\mu = \Lambda_\text{c} \approx 0.607 \text{ GeV}. \]

In the Lambert scheme [Eq. (3) with the central value $c_2 = -4.76$] there is one pole at $\mu = \Lambda_\text{c} \approx 0.262 \text{ GeV};$ the cut begins at an even lower value $\mu = \Lambda_\text{c} \approx 0.208 \text{ GeV}$. The $2 \delta \text{anQCD}$ coupling $A_1(\mu^2)$ has, of course, no Landau singularities (poles and cuts), although it almost coincides with the Lambert pQCD coupling $a_{pt}(\mu^2)$ at higher scales $|\mu^2| > 1 \text{ GeV}^2$, Ref. [34].
\[ k_{s/us} = 1.0. \] Therefore, we estimate the \( us \) part of the binding energy in (F)APT in the following way:

\[ E_{bb}(us; (F)APT) = \frac{1}{2} \left[ E_{bb}(us; Q_{s,(F)APT}^2) + (E_{bb}(us))_{\text{max}} \right] - \frac{1}{2} \left[ E_{bb}(us; Q_{s,(F)APT}^2) - (E_{bb}(us))_{\text{max}} \right]. \]  

(57)

In Eqs. (47)-(50), the uncertainties in the \( m_b \) originating from these determinations of the \( us \) binding energy are denoted by the subscript \((us)\).

The related uncertainties for the extracted values of \( m_b \) originate from the variation of the \( s/us \) separation parameter \( k_{s/us} \), and are denoted by the subscript \((s/us)\) in Eqs. (47)-(50). The parameter \( k_{s/us} \) was varied in such a way that the last [fifth, \( t_5(s) \)] term in the series for the soft mass \( M_{\Upsilon(1s)}(s) \) [cf. Eqs. (51a)-(54a)] varies between the penultimate term \( t_4(s) \) of these series, and its negative \(-t_4(s)\), these two cases correspond to the upper and the lower entry of \((s/us)\) uncertainty of \( m_b \), respectively. In the (F)APT case the exact renormalon cancellation was not achieved and the parameter \( k_{s/us} \) was varied between 0.1 and 10, i.e., \( k_{s/us} = 1.0^{+0.9}_{-0.0} \).

The other uncertainty in the determination of \( m_b \) comes from the uncertainty of the \( \Lambda \) scale. In (F)APT it comes from \( \Lambda^2 = 0.260 \pm 0.030 \text{ GeV} \) and is denoted by the subscript \((\Lambda)\) in Eq. (47a). In the \( 2\text{\&anQCD} \) model and in the two pQCD approaches (the Lambert scheme and \( \overline{\text{MS}} \) scheme), this uncertainty comes from \( \alpha_s(M_Z^2; \overline{\text{MS}}) = 0.1184 \pm 0.007 \) and is denoted by the subscript \((\alpha_s)\) in Eqs. (48a), (49a), and (50a).

Yet another uncertainty of \( m_b \), in the \( 2\text{\&anQCD} \) model and in Lambert scheme pQCD, comes from the variation of the \( \Lambda \) renormalization scheme parameter \( c_2 = -4.76^{+2.66}_{-0.97} \), cf. Table I and Eqs. (16)-(18) and is denoted in Eqs. (48a) and (49a) by the subscript \((c_2)\). The scheme in (F)APT was fixed by the underlying pQCD solution, Eqs. (9)-(10): \( c_2 = c_3 = \cdots = 0 \), i.e., effectively the two-loop solution.

The uncertainty due to the variation of the soft renormalization scale \( \mu_s \) was denoted in Eqs. (47)-(50) by the subscript \((\mu_s)\). We varied \( \mu_s^2 \) around the central value \( (Q_{s,\text{centr}}^2)^{\mu_s} \) of the soft reference scale, between \( 2(Q_{s,\text{centr}}^2)^{\mu_s} \) and \( (1/2)(Q_{s,\text{centr}}^2)^{\mu_s} \). The scale \( (Q_{s,\text{centr}}^2) \) is determined by Eqs. (36), (37) and (39) in pQCD, \( 2\text{\&anQCD} \) and (F)APT, respectively, for central values of the input parameters \( m_b, k_{s/us}, \) etc.

Finally, the uncertainty \( \delta m_b(m_c \neq 0) = \pm 0.005 \text{ GeV} \) due to nonzero \( m_c \) mass [Eq. (26) cf. also Eqs. (29)-(32)] results in the uncertainties \( \mp 0.005 \) GeV of \( m_b \), denoted in Eqs. (47)-(50) by the subscript \((m_c)\).

We see in Eqs. (47)-(50) that the largest resulting uncertainty in the determination of \( m_b \) is the one originating from the uncertainty of the determination of the \( us \) binding energy (except in (F)APT where \( |E_{bb}(us)| \) values are small). These uncertainties are larger in the two pQCD approaches, due to the influence of the nearby (unphysical) Landau singularities in the running couplings. The contribution of the \( us \) regime to the quarkonium mass, in the \( 2\text{\&anQCD} \) model and in pQCD, increases the predicted value of \( m_b \). This is so because the \( us \) binding energies are in these cases significant and negative; cf. also Fig. 3(a).

If we had ignored the existence and separation of the \( us \) contributions, i.e., if we had used in the entire binding energy \( E_{bb} \) simply a common soft renormalization scale \( \mu_s \sim Q_s \), the predicted values of \( m_b \) in the \( 2\text{\&anQCD} \) model and in Lambert and \( \overline{\text{MS}} \) pQCD would have decreased, by \(-0.068, -0.091, \) and \(-0.177 \text{ GeV} \), respectively, as can be deduced from the \( us \)-origin uncertainties in Eqs. (48a)-(50a). On the other hand, in (F)APT the choice \( \mu_s = Q_{s,(F)APT} \) would only slightly increase the central value of \( m_b \), by \(0.002 \text{ GeV} \) [cf. Eq. (47a)], basically because the values of \( |E_{bb}(us)| \) in (F)APT are much smaller; cf. Fig. 3(b).

For better visibility, we present the results for the central extracted values of \( m_b \) of the aforementioned four models in Table III and for various uncertainties \( \delta m_b \) in Table III.

| model        | \( m_b(\delta m_b) \) | \( k_{s/us} \) | \( Q_s \) | \( M_{\Upsilon(1s)}(s) \) | \( E_{bb}(us) \) | \( \delta E_{bb} \) |
|--------------|----------------------|----------------|--------|--------------------------|----------------|------------------|
| (F)APT       | 4.155(±0.022)         | 1.000          | 1.596  | 9.454                    | 0.006          | ±0.003           |
| 2\&anQCD     | 4.353(±0.084)         | 0.238          | 2.084  | 9.815                    | -0.355         | ±0.151           |
| pQCD Lambert | 4.382(±0.111)         | 0.306          | 1.729  | 9.816                    | -0.355         | ±0.201           |
| \( \overline{\text{MS}} \) | 4.505(±0.231)         | 0.248          | 1.869  | 10.078                   | -0.617         | ±0.394           |

We wish to address here briefly the question of nonperturbative (NP, higher-twist) contribution to the quarkonium mass. In the heavy quark system such as \( bb \), the NP contribution can be estimated, and in the leading order it comes from the gluon condensate and is given by

\[ E_{bb}(us)^{(NP)} \approx m_b^2 \pi^2 \frac{624}{425} \left( \frac{4\pi}{3} m_b \right)^{-4} \frac{1}{a_{pi}^2} \left( \frac{\alpha_s}{\pi} G_{\mu\nu} G^{\mu\nu} \right). \]  

(58)
TABLE III: Uncertainties $\delta m_b$ of the extracted value of $m_b$ coming from various sources: (1) from the evaluation of the $u s$ sector; (2) from the variation of the $s\sim u s$ separation parameter $k_{s/u s}$; (3) from the variation of $\alpha_s$ (or, in (F)APT: variation of $\Lambda$); (4) from the variation of the $c_2$ parameter (in $2\delta anQCD$, and in pQCD in the Lambert scheme); (5) from the variation of the soft renormalization scale $\mu_s$; (6) from the uncertainty of $(\delta m_b)_{u s}$, of Eq. (25). See the text for details.

| model | $\delta m_b (u s)$ | $\delta m_b (s/u s)$ | $(k_{s/u s})$ | $\delta m_b (\alpha_s)$ | $\delta m_b (c_2)$ | $\delta m_b (\mu_s)$ | $\delta m_b (m_b)$ |
|-------|-------------------|-------------------|------------|-------------------|-------------------|-------------------|-------------------|
| (F)APT | $+0.002$ | $+0.006$ | $(1.0+9.0)$ | $-0.019$ | $-$ | $-$ | $+0.014$ |
| $2 \delta anQCD$ | $-0.088$ | $+0.015$ | $(0.238+0.100)$ | $-0.005$ | $-0.023$ | $(-4.76+2.66)$ | $+0.017$ |
| pQCD | $-0.097$ | $-0.016$ | $(0.238+0.173)$ | $+0.005$ | $+0.034$ | $(-4.76-0.97)$ | $-0.025$ |
| Lamb. | $+0.007$ | $+0.017$ | $(0.306+0.194)$ | $+0.010$ | $+0.027$ | $(-4.76+2.66)$ | $-0.002$ |
| pQCD | $+0.091$ | $-0.013$ | $(0.306+0.119)$ | $-0.010$ | $-0.008$ | $(-4.76-0.97)$ | $-0.041$ |
| MS | $+0.200$ | $+0.084$ | $(0.248+0.181)$ | $+0.031$ | $-$ | $-$ | $-0.004$ |

The factor $1/a_{pt}^4(\mu_{us}^2)$ in (four-loop) $\overline{MS}$ pQCD is unreliable for realistic $us$ scales $\mu_{us} \approx 1$ GeV, due to the vicinity of the Landau singularities (cf. footnote 16). In the $2\delta anQCD$ model, for purposes of estimation, we replace $1/a_{pt}^4(\mu_{us}^2)$ by $1/(\Lambda_4(\mu_{us}^2))$ or by $1/(\bar{\Lambda}_4(\mu_{us}^2)).$ In the interval $(1.1$ GeV $< \mu_{us} < 1.3$ GeV) we have $\Lambda_4 \sim \bar{\Lambda}_4 \sim 10^{-4};$ the couplings $\Lambda_4$ and $\bar{\Lambda}_4$ cover in this interval the values between $0.5 \times 10^{-4}$ and $2 \times 10^{-4}.$ For these values, and using the central value of the gluon condensate $\langle (\alpha_s/\pi)G^2 \rangle = 0.009$ GeV$^2$ (cf. also Refs. 88 and 55), and for $\bar{m}_b = 4.3$ GeV, we obtain the following estimate:

$$E_{b\bar{b}}(\mu_{us})^{(NP)} = 0.05_{-0.05}^{+0.05} \text{GeV}.$$  \hspace{1cm} (59)

This effect is relatively small and has large uncertainties. If we take it into account, then the central extracted values of $m_b$ in this subsection decrease somewhat, the decrease being $\delta m_b^{(NP)} \approx -0.025$ GeV.

We wish to comment briefly on the following aspect: the results of this subsection show that the extracted values $\bar{m}_b$ and various uncertainties $\delta \bar{m}_b$ are similar in the $2\delta anQCD$ model and the corresponding Lambert pQCD. The main reason for this lies in the fact that the scheme parameters $(\epsilon_j, j \geq 2)$ are the same in both frameworks, and that the two corresponding running couplings practically merge at high momenta $|Q^2| > \Lambda^2: \Lambda_4(Q^2) - a_{pt}(Q^2) \sim (\Lambda^2/Q^2)^3.$ Nonetheless, the evaluation methods for these two cases differ somewhat due to the different types of truncations involved. In pQCD, the quantities $2m_b$ and $E_{b\bar{b}}$ were calculated as truncated series of powers $a_{pt}^n$, truncated at $a_{pt}^4$ and $a_{pt}^5$, respectively. In the $2\delta anQCD$ model, they were effectively calculated as series in logarithmic derivatives $\bar{A}_n$, truncated at $\bar{A}_4$ and $\bar{A}_5$, respectively; namely, the analytic power analogs $\bar{A}_n$ in $2m_b$ were evaluated as a series in $\bar{A}_n$’s up to $k = 4$, and in $E_{b\bar{b}}$ as a series in $\bar{A}_n$’s up to $k = 5$ (cf. Appendix A).

For comparison, we present in Table IV a list of extracted values of $m_b$ (and $m_c$) by various methods in the literature: lattice calculations, sum rules (pQCD+OPE), and from meson spectra (pQCD). The latter pQCD calculations account for the renormalon cancellation, but most of them either do not consider the ultrasoft contributions, or they include them unseparated from the soft contributions (using the same scale in the soft and the ultrasoft). We can see that (F)APT results agree with those of the usual pQCD calculations of the quarkonium spectrum and those of the sum rules (pQCD+OPE). The $2\delta anQCD$ results are incompatible with those results, but are compatible with the results of lattice calculations. The same can be claimed for the estimates of our pQCD approach (in the Lambert and $\overline{MS}$ schemes), but the uncertainties there, coming principally from the ultrasoft sector, are larger, especially in $\overline{MS}$ scheme.

B. Charm mass extraction

In this case, $q\bar{q} = c\bar{c}$, and the quarkonium mass is now $M_{J/\psi(1S)} = 3.0969$ GeV 19. We basically repeat the analysis as in the case of $b\bar{b}$. There are some differences, though:

- The relation 27 is now at $N_f = 3$; therefore, the transition to the relation at the soft renormalization scales, Eq. (29), which is also at $N_f = 3$, has now no threshold transition complication.

- The typical soft reference scales [Eqs. 30 and 38] are now significantly lower: $Q_s \approx 1$ GeV or even lower (in the $b\bar{b}$ case we had: $Q_s \approx 2$ GeV). This, in conjunction with our suggestion that the considered models $2\delta anQCD$ and pQCD (in the Lambert and $\overline{MS}$ schemes) are not necessarily to be trusted at scales below 1.1 GeV, implies that the typical soft renormalization scales $\mu_s$ should be chosen significantly higher than $Q_s$. We
choose $\mu_s^2 = (3 \pm 1)Q_s^2$ in these three models. In this case, the lowest possible soft scale, $(\mu_s)_{\text{min}} = \sqrt{2}Q_s$ is slightly above 1.1 GeV. In (F)APT, the soft renormalization scale will also be varied in this way, giving, however, somewhat lower central value for the renormalization scale: $\mu_s = \sqrt{3}Q_s, (\text{F}AP\text{T}) \approx 1.004$ GeV.\footnote{If we used in (F)APT a lower definition of the central renormalization scale, $\mu_s = Q_s, (\text{F}AP\text{T}) \approx 0.58$ GeV, the predicted central value of $\overline{m}_c$ would go up by only 0.005 GeV.} The scale variation $\mu_s^2 = (3 \pm 1)Q_s^2$ results in small uncertainties $(\delta m_c)(\mu_s)$ of the extracted mass $m_c$, but these uncertainties may be underestimated because $\mu_s^2 > Q_s^2$.

• In general, the cancellation of the leading renormalon now implies for the $s$-$us$ separation parameter $k_{s/us}$ such values for which the absolute values of $E_{cc}(us)$ are significantly smaller than in the $bb$ case, and consequently, the $us$ ambiguities are smaller. Since we now use for the central choice of the soft renormalization scale $\mu_s^2 = 3Q_s^2$, $E_{cc}(us)$ is calculated in the 2$\delta$anQCD model and in pQCD in the following way:

$$E_{cc}(us) = \frac{1}{2} \left[ E_{cc}(us; 3Q_s^2) + E_{cc}(us; 1.1^2\text{GeV}^2) \right] + \frac{1}{2} \left[ E_{cc}(us; 3Q_s^2) - E_{cc}(us; 1.1^2\text{GeV}^2) \right] ,$$

where the soft reference scale $Q_s$ in the 2$\delta$anQCD model is determined by Eq. (38)\footnote{Note that in the 2$\delta$anQCD model in the $cc$ case the condition (37) cannot be fulfilled.} and in pQCD by Eq. (36).

In (F)APT, we do not have practical problems at low scales $\mu < 1.1$ GeV, and the $us$ energy as a function of low scale $\mu_{us}$ turns out to have a moderate local maximum and a moderate local minimum; hence we use

$$E_{cc}(us; (F)AP\text{T}) = \frac{1}{2} \left[ E_{cc}(us)_{\text{max}} + E_{cc}(us)_{\text{min}} \right] + \frac{1}{2} \left[ E_{bb}(us)_{\text{max}} - E_{cc}(us)_{\text{min}} \right] ,$$

where these values are quite small: in the central case ($\overline{m}_c = 1.257, k_{s/us} = 1.0$), the local maximum is $E_{cc}(us)_{\text{max}} \approx +0.003$ GeV and is reached at $\mu_{us} \approx 0.71$ GeV, and the local minimum is $E_{cc}(us)_{\text{min}} \approx -0.006$ GeV and is reached at very low scale $\mu_{us} \approx 0.11$ GeV [cf. Fig. 3(b)].

• The exact renormalon cancellation requirement in (F)APT gives again an exceedingly small value of the $s$-$us$ separation parameter, $k_{s/us} \approx 3 \times 10^{-9}$. In (F)APT we vary the parameter $k_{s/us}$ again around its central chosen value 1.0, in the interval between 0.1 and 10.\text{x}, just as it was done in the $bb$ case of (F)APT.
In the (F)APT case, the values of \( m^\text{us} \) for the central input values of parameters \( \overline{m}_c, \mu_s \), are larger than in the 2\( \delta \)anQCD model and in pQCD in the two schemes, as a function of the ultralight scales \( \mu_{us} \), is presented in Fig. 4(a), and in the case of (F)APT in Fig. 4(b). Comparing Figs. 4(a) and (b), we see that \( |E_{cc}(us)| \sim 10^{-2} - 10^{-1} \) GeV in the 2\( \delta \)anQCD model, and \( \sim 10^{-3} \) GeV in (F)APT. Furthermore, with the corresponding curves in Figs. 4(a) and (b) for the \( bb \), we can see that in the 2\( \delta \)anQCD model and in the two pQCD approaches, the absolute values \( |E_{cb}(us)| \) are by almost two orders of magnitude smaller than \( |E_{bb}(us)| \), principally because the renormalon cancellation gives us in the two cases significantly different \( s\)-\( us \) separation parameter values: \( k_{s\!/us}(cc) = 4.06 \) and \( k_{s\!/us}(bb) = 0.238 \). Further, the values of \( |E_{q\!q}(us)| \) (for \( q = c, b \)) in pQCD are larger than in the 2\( \delta \)anQCD model, especially in \( \overline{\text{MS}} \) pQCD. In the (F)APT case, the values of \( |E_{q\!q}(us)| \) \( (q = c, b) \) are quite small, being in \( cc \) case smaller by almost one order of magnitude. All this is reflected also in the numerical results of this and of the previous subsection.

The resulting extracted values of \( \overline{m}_c \) are

\[
\overline{m}_c((F)\text{APT}) = \left\{ 1.257 \mp 0.002 \mp 0.002 \mp 0.011 \mp 0.002 \right\} \text{GeV}
\]

\[
= 1.257 \pm 0.012 \text{GeV} , \quad \text{with} : \sqrt{3}Q_s((F)\text{APT}) = 1.00 \text{GeV} , \quad k_{s\!/us} = 1.0 . \tag{62b}
\]

\[
\overline{m}_c(2\delta\text{anQCD}) = \left\{ 1.266 \mp 0.003 \mp 0.007 \mp 0.005 \mp 0.014 \mp 0.003 \right\} \text{GeV} \tag{63a}
\]

\[
= 1.266 \pm 0.017 \text{GeV} , \quad \text{with} : \sqrt{3}Q_s = 1.42 \text{GeV} , \quad k_{s\!/us} = 4.06 . \tag{63b}
\]

\[
\overline{m}_c(\text{pQCD}_{\text{Lamb}}) = \left\{ 1.265 \pm 0.001 \pm 0.021 \pm 0.004 \pm 0.003 \right\} \text{GeV} \tag{64a}
\]

\[
= 1.265 \pm 0.027 \text{GeV} , \quad \text{with} : \sqrt{3}Q_s = 1.38 \text{GeV} , \quad k_{s\!/us} = 5.59 . \tag{64b}
\]

\[
\overline{m}_c(\text{pQCD}_{\text{MS}}) = \left\{ 1.272 \mp 0.011 \mp 0.066 \mp 0.002 \mp 0.003 \right\} \text{GeV} \tag{65a}
\]

\[
= 1.272 \pm 0.078 \text{GeV} , \quad \text{with} : \sqrt{3}Q_s = 1.58 \text{GeV} , \quad k_{s\!/us} = 3.08 . \tag{65b}
\]

In order to see more clearly the renormalon cancellation, we present below, as in Sec. [IV A] the sum for the soft mass \( M_{J/\psi(1S)}(s) = 2m_c + E_{cc}(s) \), combining in each parenthesis the (positive) term \( a^n \) from \( 2m_c \) and the (negative) term \( a^{n+1} \) from the soft binding energy \( E_{cc}(s) \) \( (n = 0, 1, \ldots, 4) \), for the central input values of parameters \( \overline{m}_c, \mu_s \).
TABLE V: Extracted central values of $\overline{m}_c$ in the four models, for the central input parameter values (with the total uncertainties $\delta \overline{m}_c$). Included are the corresponding input parameter $k_s/\text{us}$, and the resulting scales: soft renormalization scale $\mu_s = \sqrt{3} Q_s$; soft mass $M_{J/\psi(1S)}(s)$; averaged ultrasonic energy $E_{cc}(us)$ and its ambiguity $\delta E_{cc}(us)$ [cf. Eqs. (58)-(61)]. All scales are given in GeV. Note that $M_{J/\psi(1S)}(s) + E_{cc}(us) = 3.097 \text{ GeV}$, i.e., the physical mass $M_{J/\psi(1S)}$.

| model       | $\overline{m}_c$ (GeV) | $k_s/\text{us}$ | $\sqrt{3} Q_s$ | $M_{J/\psi(1S)}(s)$ | $E_{cc}(us)$ | $\delta E_{cc}$ |
|-------------|------------------------|-----------------|----------------|---------------------|--------------|-----------------|
| (F) APT     | 1.257(±0.012)          | 1.001           | 1.004          | 3.098               | -0.001       | ±0.004          |
| 2δanQCD     | 1.266(±0.017)          | 4.06            | 1.422          | 3.087               | +0.010       | ±0.006          |
| pQCD Lamb.  | 1.265(±0.027)          | 5.59            | 1.382          | 3.083               | +0.013       | ±0.003          |
| pQCD $\overline{M}_S$ | 1.272(±0.078) | 3.08 | 1.585 | 3.131 | -0.034 | ±0.024 |

TABLE VI: Uncertainties $\delta \overline{m}_c$ of the extracted value of $\overline{m}_c$ coming from various sources: (1) from the evaluation of the $\text{us}$ sector; (2) from the variation of the $s$-$\text{us}$ separation parameter $k_s/\text{us}$; (3) from the variation of $\alpha_s$ (or, in (F)APT: variation of $\Lambda$); (4) from the variation of the $c_2$ parameter (in 2δanQCD, and in pQCD in the Lambert scheme); (5) from the variation of the soft renormalization scale $\mu_s$. See the text for details.

| model       | $\delta \overline{m}_c$ (us) | $\delta \overline{m}_c$ (s/us) | $\delta \overline{m}_c$ ($k_s/\text{us}$) | $\delta \overline{m}_c$ ($\alpha_s$) | $\delta \overline{m}_c$ ($c_2$) | $\delta \overline{m}_c$ ($\mu_s$) |
|-------------|------------------------------|---------------------------------|----------------------------------------|---------------------------------|-------------------------------|------------------------------|
| (F) APT     | -0.002                       | -0.002                          | (1.49-9.0)                             | -0.011                          | -                             | -0.002                      |
| 2δanQCD     | +0.003                       | +0.007                          | (4.06-3.61)                            | -0.005                          | -0.014                        | -0.002                      |
| pQCD Lamb.  | -0.003                       | -0.007                          | (4.06+39.5)                            | +0.005                          | +0.003                        | +0.005                      |
| pQCD $\overline{M}_S$ | -0.011                       | -0.066                          | (3.08-2.86)                            | -0.004                          | 0.000                         | -0.003                      |

($= \sqrt{3} Q_s$) and $k_s/\text{us}$; separately we present below also $E_{cc}(us)$.

$$M_{J/\psi(1S)}(s; \text{(F)APT}) = 2.513 + (0.409 - 0.056) + (0.228 - 0.082) + (0.133 - 0.071) + (0.046 - 0.023) \text{ GeV}$$

$$= 2.513 + 0.354 + 0.146 + 0.062 + 0.023 \text{ GeV} (= 3.098 \text{ GeV}) ,$$ (66a)

$$E_{cc}(us; \text{(F)APT}) = -0.001 \pm 0.004 \text{ GeV} , \quad (\overline{m}_c = 1.257 \text{ GeV}, \, k_s/\text{us} = 1.0) ;$$ (66b)

$$M_{J/\psi(1S)}(s; 2\delta\text{anQCD}) = 2.531 + (0.349 - 0.053) + (0.328 - 0.171) + (0.253 - 0.150) + (0.979 - 0.979) \text{ GeV}$$

$$= 2.531 + 0.296 + 0.157 + 0.103 + 0.000 \text{ GeV} (= 3.087 \text{ GeV}) ,$$ (67a)

$$E_{cc}(us; 2\delta\text{anQCD}) = 0.010 \mp 0.006 \text{ GeV} , \quad (\overline{m}_c = 1.266 \text{ GeV}, \, k_s/\text{us} = 4.06) ;$$ (67b)

$$M_{J/\psi(1S)}(s; \text{pQCDLamb.}) = 2.530 + (0.354 - 0.061) + (0.303 - 0.141) + (0.404 - 0.305) + (0.662 - 0.662) \text{ GeV}$$

$$= 2.530 + 0.293 + 0.161 + 0.099 + 0.000 \text{ GeV} (= 3.083 \text{ GeV}) ,$$ (68a)

$$E_{cc}(us; \text{pQCDLamb.}) = 0.013 \mp 0.003 \text{ GeV} , \quad (\overline{m}_c = 1.265 \text{ GeV}, \, k_s/\text{us} = 5.59) ;$$ (68b)

$$M_{J/\psi(1S)}(s; \text{pQCD$\overline{M}_S$}) = 2.544 + (0.368 - 0.066) + (0.348 - 0.163) + (0.455 - 0.356) + (0.778 - 0.778) \text{ GeV}$$

$$= 2.544 + 0.302 + 0.185 + 0.099 + 0.000 \text{ GeV} (= 3.131 \text{ GeV}) ,$$ (69a)

$$E_{cc}(us; \text{pQCD$\overline{M}_S$}) = -0.034 \pm 0.024 \text{ GeV} , \quad (\overline{m}_c = 1.272 \text{ GeV}, \, k_s/\text{us} = 3.08) ;$$ (69b)

As in the previous subsection in the case of $b\bar{b}$, we present now for the case $c\bar{c}$, for better visibility, the results for the central extracted values of $\overline{m}_c$ of the four models in Table V and for various uncertainties $\delta \overline{m}_c$ in Table VI.

The nonperturbative (NP) contribution coming from the gluon condensate, cf. Eq. (58) for the $b\bar{b}$ system in the previous subsection, is unreliable for the lighter $c\bar{c}$ system, since the next-to-leading corrections are in this case large and tend to make the result unreliable, cf. Ref. [100].

Comparing the results for $\overline{m}_c$ in this subsection with those for $\overline{m}_b$ in the previous subsection, we see that the soft-ultrasonic separation parameter $k_s/\text{us}$ in the 2δanQCD model and pQCD is now larger: $k_s/\text{us} \approx 3-5$, while in $\overline{m}_b$
case we had $k_{\text{susy}} \approx 0.2-0.3$. This is a consequence of the requirement of the leading renormalon cancellation. As a result, the ultrasoft contributions to the $J/\psi(1S)$ mass are by an order of magnitude smaller (in absolute value) than those to the $\Upsilon(1S)$ mass, surprisingly. The extracted values of $m_\tau$ thus suffer from less (ultrasoft) uncertainty than the extracted values of $m_b$. On the other hand, in (F)APT, the ultrasoft sector is always suppressed, a consequence of the suppressed (F)APT couplings in the infrared.

The extracted values of $m_c$ obtained in this work, in all four models, are compatible with all those obtained in the literature (from lattice, sum rules, and spectrum calculations), as can be seen from Table IV.

V. SUMMARY

We evaluated, in two analytic QCD models and in perturbative QCD (pQCD, in two schemes), the quark-antiquark binding energies (up to N$^3$LO) and masses of ground state $q\bar{q}$ quarkonia ($q = b, c$), as functions of the quark mass $m_q \equiv m_q(\mu^2 = m_q^2)$, also called the $\overline{\text{MS}}$ quark mass. In analytic QCD models the QCD running coupling $A_1(Q^2)$ has no unphysical (Landau) singularities in the $Q^2$ plane.

The use of the analytic QCD models was motivated by the fact that the typical soft ($s$) momentum scales $Q_s$ in the ground bound states of quarkonia are low ($Q_s \approx 2$ GeV and 1 GeV, for $b\bar{b}$ and $c\bar{c}$, respectively), and that the typical ultrasoft ($u$) momentum scales $Q_{us}$ are even lower. This, in conjunction with the fact that Landau singularities of the pQCD coupling $a_{\text{pt}}(Q^2)$ reach relatively high momenta: $Q \approx 0.61$ GeV in the usual (four-loop) $\overline{\text{MS}}$ scheme (with $c_2 \equiv \beta_3/\beta_0 = 4.471$), and $Q \approx 0.26$ GeV in the Lambert scheme ($c_2 = -4.76$). So we can apply in analytic QCD generally more natural renormalization scales at which the pQCD couplings are sometimes “out of control.”

One analytic QCD model applied here was the Analytic Perturbation Theory (APT) of Shirkov, Solovtsov, Solovtsova, and Milton et al. (Refs. [34, 35]), which has been extended by Bakulev, Mikhailov and Stefanis to the Fractional Analytic Perturbation Theory (FAPT) for calculation of the fractional power analogs (Refs. [40, 42, 43]). (F)APT can be regarded as a model with minimal analytization of pQCD in the conceptual sense. Namely, it keeps the perturbative discontinuity function $\rho_1^{(\text{pt})}(\sigma) \equiv \text{Im} a_{\text{pt}}(Q^2 = -\sigma - i\epsilon)$ unchanged on the entire positive-$\sigma$ semiaxis, while removing the (perturbative) discontinuity at $\sigma < 0$ in order to ensure the analyticity of $A_1^{(\text{APT})}(Q^2)$. It thus contains no additional regulators in the positive $\sigma$-range. One of the strengths of (F)APT is that it has as a parameter only the pQCD-type $\Lambda$ scale; i.e., it contains no new parameters. As a result, it has finite coupling $A_1^{(\text{APT})}(Q^2)$ at $|Q^2| \to 0$, and $A_1^{(\text{APT})}(Q^2) = a_{\text{pt}}(Q^2) \sim (\Lambda^2/Q^2)^{\delta}$ at $|Q^2| > \Lambda^2$. The latter means that it behaves somewhat differently from the underlying pQCD (with the same $\Lambda$) even at high squared momenta $|Q^2|$. The value of the scale $\Lambda$ is adjusted so that the high-$|Q^2|$ QCD phenomenology is reproduced.

The other analytic QCD model applied here was the two-delta analytic QCD model ($2\delta$anQCD), Refs. [34, 35]. This model can be regarded as a model with minimal analytization of pQCD in the numerical sense. Namely, in this model the behavior of the discontinuity function $\rho_1^{(\text{2}\delta)}(\sigma) \equiv \text{Im} A_1^{(\text{2}\delta)}(-\sigma - i\epsilon)$ in the unknown low-$\sigma$ regime ($0 \leq \sigma \lesssim 1$ GeV) is parametrized (with two deltas) in such a way that: (a) at $|Q^2| > \Lambda^2$ the model becomes practically indistinguishable from the (underlying) pQCD, $A_1^{(\text{2}\delta)}(Q^2) - a_{\text{pt}}(Q^2) \sim (\Lambda^2/Q^2)^{\delta}$; and (b) the measured value of the semihadronic strangeless $V + A$ decay ratio of the $\tau$ lepton (the hitherto best measured inclusive low-energy QCD observable), $r_\tau \approx 0.203$, is reproduced. These conditions fix most of the mentioned low-$\sigma$ regime parameters. The value of the scale $\Lambda$ is the same as in the (underlying) pQCD, so that the high-$|Q^2|$ QCD phenomenology is reproduced. In contrast with (F)APT, in the 2$\delta$anQCD model one relevant parameter remains variable, namely the parameter $c_2 (\equiv \beta_3/\beta_0)$, which we vary in the phenomenologically viable interval, i.e., approximately $-6 < c_2 < -2$.

The main conclusions of this work are the following: analytic QCD approaches which at high energies follow the pQCD behavior closely (such as the 2$\delta$anQCD model) indicate that the ultrasoft regime in the $\Upsilon(1S)$ quarkonium ($b\bar{b}$) is important. Our approach, together with the leading renormalon cancellation condition, gives us clues about how to estimate the effects of the ultrasoft regimes in pQCD. In both the 2$\delta$anQCD model and in pQCD we obtain, as a consequence, extracted values of $m_b$ which are significantly higher ($m_b \geq 4.3$ GeV) than most of those ($m_b \approx 4.2$ GeV) obtained in the sum rule approaches (which use pQCD+OPE) and in the usual pQCD calculations of meson spectra. These approaches usually either do not include the ultrasoft contributions, or they include them unseparated from the soft contributions (i.e., the ultrasoft and soft scales are set to be equal). As an additional consequence, the uncertainties in the extracted values of $m_b$ in our approach are dominated by the ultrasoft sector and are, especially in pQCD in the $\overline{\text{MS}}$ scheme, larger than in the usual pQCD approaches. Further, the extracted values of $m_\tau$ in the 2$\delta$anQCD model, $m_\tau \approx (4.35 \pm 0.08)$ GeV, are compatible with those of lattice calculations; cf. Table IV. On the other hand, the 2$\delta$anQCD model indicates that the ultrasoft regime in the $J/\Psi(1S)$ quarkonium ($c\bar{c}$) is less important, principally because the leading renormalon cancellation condition results in smaller ultrasoft coefficients in this system. The extracted values, $m_c \approx (1.27 \pm 0.02)$ GeV, are compatible with those of pQCD (or pQCD+OPE) approaches, and those of the other hand, the (F)APT of Shirkov et al., suppresses the
infrared contributions because the higher order couplings in (F)APT are more strongly suppressed in the infrared than the $2\delta\alpha$nnQCD couplings. The extracted values in (F)APT, $\overline{m}_b \approx (4.16 \pm 0.02)$ GeV and $\overline{m}_c \approx (1.26 \pm 0.01)$ GeV, are compatible with those obtained from the sum rules and from the usual pQCD spectrum calculations.

Acknowledgments

We thank A. Pineda for useful comments. C.A. thanks Bogolyubov Laboratory of Theor. Physics, of the Joint Institute for Nuclear Research, Dubna, for warm hospitality during part of this work. C.A. further thanks J. Otálora for help in using calculational software. This work was supported in part by MECESUP2 (Chile) Grant FSM 0605-D3021 (C.A.), and by FONDECYT (Chile) Grant No. 1095196 and Anillos Project ACT119 (G.C.).

Appendix A: Analytic analogs of powers $a_{pt}^\nu$ and of terms $a_{pt}^\nu \ln^k a_{pt}$ in general analytic QCD models

We consider that a (general) anQCD model is defined via an analytic analog $A_1(Q^2)$ of $a_{pt}(Q^2)$ in their complex plane, or, equivalently, by the discontinuity function $\rho_1(\sigma) \equiv \text{Im} \ A_1(-\sigma - i\epsilon)$ on the positive semiaxis $\sigma > 0$.

For such general anQCD models, the higher order couplings $A_\nu(Q^2)$ [analogs of $a_{pt}^\nu(Q^2)$] were constructed in Refs. [22, 23] for integer $\nu$, and Ref. [46] for general (noninteger) $\nu$. Below we will summarize the basic aspects of such construction.

Since the general anQCD models, with the exception of APT, have at low $\sigma \left( \lesssim 1 \text{ GeV}^2 \right)$ different discontinuity function than the pQCD coupling $a_{pt}(Q^2)$, we cannot use the (F)APT method [Eq. (3)] for the construction of the analogs of $a_{pt}^\nu \ln^k a_{pt}$. The analogs of the integer powers $a_{pt}^\nu$ in such general models were constructed in Refs. [22, 23], where it was shown that it is imperative to construct first the analogs of the logarithmic derivatives of $a_{pt}$ in the following way:\textsuperscript{19}

\[
\left( \frac{\partial^k a_{pt}(Q^2)}{\partial (\ln Q^2)^k} \right)_{\text{an}} \equiv \frac{\partial^k A_1(Q^2)}{\partial (\ln Q^2)^k} \quad (k = 0, 1, 2, \ldots).
\]

(A1)

In pQCD, the logarithmic derivatives

\[
\bar{a}_{pt,k+1}(Q^2) \equiv \frac{(-1)^k}{\beta_0^k k!} \frac{\partial^k a_{pt}(Q^2)}{\partial (\ln Q^2)^k}, \quad (k = 0, 1, 2, \ldots),
\]

(A2)

are related with the powers of $a_{pt} \equiv \alpha_s/\pi$ in the following way (using RGEs in pQCD):

\[
\begin{align*}
\bar{a}_{pt,2} &= a_{pt}^2 + c_1 a_{pt}^3 + c_2 a_{pt}^4 + c_3 a_{pt}^5 + \cdots, \\
\bar{a}_{pt,3} &= a_{pt}^3 + \frac{5}{2} c_1 a_{pt}^4 + \left( 3c_2 + \frac{5}{2} c_1^2 \right) a_{pt}^5 + \cdots, \\
\bar{a}_{pt,4} &= a_{pt}^4 + \frac{13}{3} c_1 a_{pt}^5 + \cdots, \quad \bar{a}_{pt,5} = a_{pt}^5 + \cdots, \quad \text{etc.}
\end{align*}
\]

(A3a)

(A3b)

(A3c)

This means that the powers of $a_{pt}$ are linear combinations of logarithmic derivatives

\[
\begin{align*}
a_{pt}^2 &= \bar{a}_{pt,2} - c_1 \bar{a}_{pt,3} + \left( \frac{5}{2} c_1^2 - c_2 \right) \bar{a}_{pt,4} + \left( -\frac{28}{3} c_1^3 + \frac{22}{3} c_1 c_2 - c_3 \right) \bar{a}_{pt,5} + \cdots, \\
a_{pt}^3 &= \bar{a}_{pt,3} - \frac{5}{2} c_1 \bar{a}_{pt,4} + \left( \frac{28}{3} c_1^2 - 3c_2 \right) \bar{a}_{pt,5} + \cdots, \\
a_{pt}^4 &= \bar{a}_{pt,4} - \frac{13}{3} c_1 \bar{a}_{pt,5} + \cdots, \quad a_{pt}^5 = \bar{a}_{pt,5} + \cdots, \quad \text{etc.}
\end{align*}
\]

(A4a)

(A4b)

(A4c)

\textsuperscript{19} If the analytization is performed in any other way, the renormalization scale and scheme dependence of the resulting truncated analytic series of any observable $D(Q^2)$ will in general increase (instead of decrease) when the number of terms in the series increases; cf. [22, 23].
These relations, in conjunction with the analytization Eq. [A1], imply that the analytic analogs \( A_k \) of powers \( a_{pt}^k \), in general anQCD models, can be expressed as linear combinations of the logarithmic derivatives

\[
\tilde{A}_{k+1}(\mu^2) = \frac{(-1)^k}{\beta_0^k k!} \frac{\partial^k A_1(\mu^2)}{\partial (\ln \mu^2)^k}, \quad (k = 1, 2, \ldots).
\]

(A5)

in the following form:

\[
\begin{align*}
A_2 &= \tilde{A}_2 - c_1 \tilde{A}_3 + \left( \frac{5}{2} c_2 - c_2 \right) \tilde{A}_4 + \left( -\frac{28}{3} c_1^3 + \frac{22}{3} c_1 c_2 - c_3 \right) \tilde{A}_5 + \cdots, \\
A_3 &= \tilde{A}_3 - \frac{5}{2} c_1 \tilde{A}_4 + \left( \frac{28}{3} c_1^2 - 3 c_2 \right) \tilde{A}_5 + \cdots, \\
A_4 &= \tilde{A}_4 - \frac{13}{3} c_1 \tilde{A}_5 + \cdots, \quad A_5 = \tilde{A}_5 + \cdots, \quad \text{etc.}
\end{align*}
\]

(A6a)

(A6b)

(A6c)

In Ref. [46] this analytization was extended to the case when \( k \mapsto \nu \) is noninteger\(^{20}\)

\[
\tilde{A}_{\nu+1}(Q^2) = \frac{1}{\pi \beta_0^\nu (\nu + 1)} \int_0^\infty \frac{d\sigma}{\sigma} \rho_1(\sigma) \text{Li}_{-\nu} \left( -\frac{\sigma}{Q^2} \right) \quad (1 < \nu),
\]

(A7)

where, as always, \( \rho_1(\sigma) \equiv \text{Im} A_1(Q^2 = -\sigma - i\epsilon) \), and \( \text{Li}_{-\nu}(z) \) is the polylogarithm function.\(^{21}\) The corresponding analogs of powers \( a_{pt}^\nu \) are then obtained by using the general relations

\[
a_{pt}^\nu = \tilde{a}_{pt,\nu} + \sum_{m=1}^{\infty} \tilde{k}_m(\nu) \tilde{a}_{pt,\nu+m}.
\]

(A8)

and the linearity of analytization, i.e.

\[
A_{\nu}(Q^2) \equiv (a_{pt}^\nu(Q^2))_{an} = \tilde{A}_{\nu}(Q^2) + \sum_{m \geq 1} \tilde{k}_m(\nu) \tilde{A}_{\nu+m}(Q^2) \quad (1 < \nu).
\]

(A9)

The coefficients \( \tilde{k}_m(\nu) \), for general real \( \nu \) and positive integer \( m \), were calculated in Ref. [46], and are combinations of gamma functions and their derivatives, with arguments involving \( \nu + \ell (\ell \) being various integers).

Furthermore, since \( a_{\nu}^k \ln^k a = \partial^k a_{\nu}/\partial a^k \), the linearity of analytization then implies

\[
A_{\nu,k}(Q^2) \equiv \left( a_{pt}^\nu(Q^2) \ln^k a_{pt}(Q^2) \right)_{an} = \frac{\partial^k A_{\nu}(Q^2)}{\partial a^k} = \frac{\partial^k}{\partial a^k} \left[ A_{\nu}(Q^2) + \sum_{m \geq 1} \tilde{k}_m(\nu) \tilde{A}_{\nu+m}(Q^2) \right] \quad (1 < \nu),
\]

(A10)

where in the terms on the right-hand side we use expressions for \( \tilde{A}_{\nu+m}(Q^2) \) obtained by Eq. (A7). Comparing Eqs. (A10) and (A7), we see that the terms in the above sum represent integrals over the scale \( \sigma \) involving the basic discontinuity function of the model (\( \rho_1 \)) and derivatives of the polylogarithm function \( \text{Li}_{-\nu-m+1} \) with respect to its index \( \nu \). In the evaluation of the binding energy \( E_{q\bar{q}} \) we will encounter the logarithmic terms of the type (A10) with \( \nu \) integer (\( \nu = n \)); however, the derivatives with respect to index \( \nu \) in Eq. (A10) imply that we must know the behavior of \( \tilde{A}_{\nu} \) around the integer value \( \nu = n \), i.e., we need to use here the expression (A7) for noninteger \( \nu \), or a version of it with improved integration convergence, Eq. (22) of Ref. [46] (cf. also the earlier footnote [20]).

**Appendix B: Ground state quark-antiquark binding energy**

According to Refs. [7] [62] [68], the perturbation expansion of the quark-antiquark binding energy \( E_{q\bar{q}} \), in terms of the quark pole mass \( m_q \equiv m \) and \( \alpha_s(\mu^2) \equiv \alpha_s \), is

\[20\] This relation was also reformulated so as to be applicable in a larger \( \nu \) interval: \(-2 < \nu\); cf. Eq. (22) of Ref. [46].

\[21\] In Mathematica [53] it is implemented under the name PolyLog[\(-\nu, z\)].
\[ E_{q\bar{q}} = E_C^\delta + \delta E_1^{(1)} + \delta E_1^{(2)} + \delta E_1^{(3)}, \quad \text{(B1)} \]

where

\[ E_C^\delta = -\frac{1}{4} \alpha_s^2 C_F^2 m, \quad \text{(B2)} \]

\[ \delta E_1^{(1)} = E_C^\delta \frac{4\alpha_s}{\pi} \left[ \beta_0(L_\mu + 1) + \frac{a_1}{8} \right], \quad \text{(B3)} \]

\[ \delta E_1^{(2)} = E_C^\delta \frac{\alpha_s^2}{\pi^2} \left\{ 12\beta_0^2 L_\mu^2 + (16\beta_0^2 + 3a_1 \beta_0 + 4\beta_1) L_\mu + \beta_0^2 \left( 4 + \frac{2\pi^2}{3} + 8\zeta(3) \right) + \left( 2a_1 \beta_0 + 4\beta_1 + \frac{a_1^2}{16} + \frac{a_2}{8} \right) + C_A C_F \pi^2 + \pi^2 C_F^2 \left( \frac{21}{16} - \frac{2}{3} S(1 + S) \right) \right\}, \quad \text{(B4)} \]

\[ \delta E_1^{(3)} = \delta E_1^{(3)} |_{\beta(\alpha_s)=0} + \delta E_1^{(3)} |_{\beta(\alpha_s)}. \quad \text{(B5)} \]

The two contributions to \( \delta E_1^{(3)} \) are

\[ \delta E_1^{(3)} |_{\beta(\alpha_s)=0} = -E_C^\delta \frac{\alpha_s^2}{\pi} \left\{ -\frac{a_1 a_2 + a_3}{32\pi^2} + a_1 \left[ -\frac{C_A C_F}{2} \right] + C_F^2 \left( -\frac{19}{16} + \frac{S(1 + S)}{2} \right) \right\} + C_A^3 \left( \frac{1}{36} + \frac{L_\mu}{6} + \frac{\ln|2|}{6} \right) + C_F^2 \left( -\frac{49}{36} + \frac{4}{3} L_\mu + \ln|2| \right) + C_A C_F \left( \frac{5}{72} + \frac{37L_\mu}{6} + \left( \frac{85}{54} - \frac{7}{6} L_\mu \right) S(1 + S) + \frac{10\ln|2|}{3} \right) + C_F^3 \left( \frac{50}{9} + 3L_\mu - \frac{S(1 + S)}{3} + \frac{8\ln|2|}{3} \right) + C_F^2 N T_F \left( \frac{11}{18} - \frac{10}{27} S(1 + S) \right) + \frac{2}{3} C_F^3 L_\mu^E \right\}, \quad \text{(B6)} \]

\[ \delta E_1^{(3)} |_{\beta(\alpha_s)} = E_C^\delta \frac{\alpha_s^3}{3^2 \pi^3} \left\{ \frac{32\beta_0^3 L_\mu^3}{3^2 \pi^2} + \left[ 12a_1 \beta_0 + 40\beta_0^3 + 28\beta_0 \beta_1 \right] L_\mu^2 + 10a_1 \beta_0^3 + 3a_1 \beta_1 + 4\beta_2 + \beta_0 \left( \frac{a_1^2}{2} + a_2 + 40\beta_1 + 8C_A C_F \pi^2 \right) + C_F^2 \left( \frac{21\pi^2}{2} - 16 \frac{\pi^2 S(1 + S)}{3} \right) + \beta_0^3 \left( \frac{16\pi^2}{3} + 64\zeta(3) \right) \right\} + \beta_0^3 \left( -8 + 4\pi^2 + \frac{2\pi^4}{45} \right)^2 + 64\zeta(3) - 8\pi^2 \zeta(3) + 96\zeta(5) \right) \left[ \left( \frac{2\pi^2}{3} + 8\zeta(3) \right) + \beta_0 \left( -\frac{a_1^2}{8} + \frac{a_2}{4} \right) \right] + C_A C_F \left( 6\pi^2 - \frac{2\pi^4}{3} \right) + C_F^2 \left( 8\pi^2 - \frac{4\pi^4}{3} + \left( -\frac{4\pi^2}{3} + \frac{4\pi^4}{9} \right) S(1 + S) \right) + \beta_1 \left( 8 + \frac{7\pi^2}{3} + 16\zeta(3) \right) \right\} + 2a_1 \beta_1 + 4\beta_2 \right\}. \quad \text{(B7)} \]

The following notations were used:

\[ L_\mu = \ln \left[ \frac{\mu}{\alpha_s C_F m} \right], \quad L_\mu = -\ln \left[ C_F \alpha_s \right], \quad L_F^E = -81.5379, \quad S = \text{spin}(=1), \quad \text{(B8)} \]

\[ C_A = 3, \quad C_F = 4/3, \quad T_F = 1/2. \quad \text{(B9)} \]
The RGE coefficients $\beta_j$ are in the $\overline{\text{MS}}$ scheme

$$
\begin{align*}
\beta_0 &= \frac{1}{4} \left( 11 - \frac{2}{3} N_f \right) , \\
\beta_1 &= \frac{1}{16} \left( 102 - \frac{38}{3} N_f \right) , \\
\beta_2 &= \frac{1}{64} \left( \frac{2857}{2} - \frac{5033}{18} N_f + \frac{325}{54} N_f^2 \right) , \\
\beta_3 &= \frac{1}{256} \left[ \frac{149753}{6} + \frac{1093}{729} N_f^3 + 3564 \zeta(3) + N_f^2 \left( \frac{50065}{162} + \frac{6472 \zeta(3)}{81} \right) - N_f \left( \frac{1078361}{162} + \frac{6508 \zeta(3)}{27} \right) \right] .
\end{align*}
$$

The constants $a_1$ and $a_2$ are

$$
\begin{align*}
a_1 &= \frac{1}{9} (31 C_A - 20 N_f T_F) , \\
a_2 &= \frac{400 N_f^2 T_F^2}{81} - C_F N_f T_F \left( \frac{55}{3} - 16 \zeta(3) \right) + C_A^2 \left( \frac{4343}{162} + \frac{1}{4} (16\pi^2 - \pi^4) + \frac{22 \zeta(3)}{3} \right) \\
&\quad - C_A N_f T_F \left( \frac{1798}{81} + \frac{56 \zeta(3)}{3} \right) .
\end{align*}
$$

The value for the constant $a_3$ associated with the three-loop soft contribution was obtained in Refs. \cite{5, 6} and is

$$
a_3 = a_3^{(0)} + a_3^{(1)} N_f + a_3^{(2)} N_f^2 + a_3^{(3)} N_f^3 ,
$$

where

$$
\begin{align*}
a_3^{(0)} &= 502.24 C_A^3 - 136.39 \left( \frac{N_C}{48} \left( N_C^2 + 6 \right) \right) , \\
a_3^{(1)} &= -709.71 C_A^2 T_F + \left( -\frac{71281}{162} + 264 \zeta(3) + 80 \zeta(5) \right) C_A C_F T_F \\
&\quad + \left( \frac{286}{9} + 296 \frac{\zeta(3)}{3} - 160 \zeta(5) \right) C_F^2 T_F - 56.83 \left( \frac{18 - 6 N_C^2 + N_C^3}{96 N_C^2} \right) , \\
a_3^{(2)} &= C_F T_F \left( \frac{14002}{81} - \frac{416 \zeta(3)}{3} \right) + C_A T_F \left( \frac{12541}{243} + \frac{64 \pi^2}{135} + \frac{368 \zeta(3)}{3} \right) , \\
&\quad a_3^{(3)} = -8000 T_F^3 .
\end{align*}
$$

**Appendix C: Renormalon-based estimate of $\sim a_{\text{pt}}^4$ coefficient**

The term $r_3$ in the expansion of $m_q/m_q$ in Eq. \cite{27} can be estimated by a method closely related with the approach presented in Sec. II of Ref. \cite{28}. The pQCD version of the sum in Eq. \cite{27} can be reexpressed in terms of $a_{\text{pt}}(\mu^2)$ at any other renormalization scale $\mu^2$

$$
S \equiv \frac{m_q}{m_q} - 1 = \frac{4}{3} a_{\text{pt}}(\mu^2) \left[ 1 + a_{\text{pt}}(\mu^2) r_1(\mu^2) + a_{\text{pt}}^2(\mu^2) r_2(\mu^2) + O(a_{\text{pt}}^3) \right] ,
$$

$$
\begin{align*}
r_1(\mu^2) &= \kappa_1 + \beta_0 L_m(\mu^2) , \\
r_2(\mu^2) &= \kappa_2 + (2 \kappa_1 \beta_0 + \beta_1) L_m(\mu^2) + \beta_0^2 L_m^2(\mu^2) , \\
(4/3) \kappa_1 &= 6.248 \beta_0 - 3.739 , \\
(4/3) \kappa_2 &= 23.497 \beta_0^2 + 6.248 \beta_1 + 1.019 \beta_0 - 29.94 ,
\end{align*}
$$

where $L_m(\mu^2) = \ln(\mu^2/m_q^2)$, while $\beta_0(N_f)$ and $\beta_1(N_f)$ are the renormalization scheme independent coefficients \cite{5, 6}. Here, $N_f = N_f$ is the number of light active flavors (quarks with masses lighter than $m_q$).

Since $r_1$ and $r_2$ are explicitly known, the Borel transform $B_S(b)$ is known to order $\sim b^2$

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

The function $B_S(b)$ has renormalon singularities at $b = 1/2, 3/2, 2, \ldots, -1/2$, \cite{101, 102, 103}. The behavior of $B_S$ near the leading infrared (IR) renormalon singularity $b = 1/2$ is determined by the resulting renormalon ambiguity of $m_q$. This ambiguity $\delta m_q$ is a (QCD) scale which, having the dimension of energy and being renormalization scale
and scheme independent, must be proportional to the QCD scale $\Lambda_{\text{QCD}}$: $\delta m_q = const \times \Lambda_{\text{QCD}} [104]$. This scale can be expressed in terms of $a_{\text{pt}}(\mu^2)$ and $\mu$ ($\mu$ being any renormalization scale) in the form

$$\Lambda = const \times \mu \exp \left( -\frac{1}{2\beta_0 a_{\text{pt}}(\mu)} \right) a_{\text{pt}}(\mu)^{-\nu} c_1^{-\nu} \left[ 1 + \sum_{k=1}^{\infty} (2\beta_0)^k (\nu - 1) \cdots (\nu - k + 1) \tilde{c}_k a_{\text{pt}}^k(\mu) \right], \quad (C3)$$

where

$$\nu = \frac{c_1}{2\beta_0} = \frac{\beta_1}{2\beta_0^2}, \quad (C4a)$$

$$\tilde{c}_1 = \frac{(c_1^2 - c_2)}{(2\beta_0)^2 \nu}, \quad \tilde{c}_2 = \frac{1}{2(2\beta_0)^4 \nu (\nu - 1)} [(c_1^2 - c_2)^2 - 2\beta_0(c_1^3 - 2c_1c_2 + c_3)] \quad (C4b)$$

$$\tilde{c}_3 = \frac{1}{6(2\beta_0)^6 \nu (\nu - 1)(\nu - 2)} [(c_1^2 - c_2)^3 - 6\beta_0(c_1^2 - c_2)(c_1^3 - 2c_1c_2 + c_3) + 8\beta_0^3(c_1^4 - 3c_1^2c_2 + c_2^2 + 2c_1c_3 - c_4)] \quad (C4c)$$

The above constants, expressed in terms of $\beta_0$ and of $c_j = \beta_j / \beta_0$, appear in the expansion of the residue of the Borel transform $B_S(b; \mu)$ at the pole $b = 1/2$

$$B_S(b; \mu) = N_m \pi \frac{\mu}{m_q(1 - 2b)^{1+\nu}} \left[ 1 + \sum_{k=1}^{\infty} \tilde{c}_k (1 - 2b)^k \right] + B_S^{(\text{an})}(b; \mu), \quad (C5)$$

where $B_S^{(\text{an})}(b; \mu)$ is analytic on the disk $|b| < 1$ and can be expanded in powers of $b$. The form of the representation $[C5]$ is called bilocal and was proposed in Ref. [77]. We can assume that the coefficients $\tilde{c}_k$ are known up to $k = 3$, because the coefficient $c_4 = \beta_4 / \beta_0$ (in the $\overline{\text{MS}}$ scheme) is known to a large degree by Padé-related methods of Ref. [105]

$$\beta_4 = \frac{1}{4^6}(A_4 + B_4N_f + C_4N_f^2 + D_4N_f^3 + E_4N_f^4) \quad (C6)$$

with $A_4 = 7.59 \times 10^5$, $B_4 = -2.19 \times 10^5$, $C_4 = 2.05 \times 10^4$, $D_4 = -49.8$, and $E_4 = -1.84$. This gives $c_4 = 123.7$ for $N_f = 3$, $c_4 = 97.2$ for $N_f = 4$, and $c_4 = 86.2$ for $N_f = 5$. The residue parameter $N_m$ can be determined with high precision by using the idea of Refs. [106], i.e., by calculating (cf. Refs. [76, 77, 107]):

$$N_m = \frac{\pi}{\mu} \frac{1}{\pi} R_S(b = 1/2), \quad (C7)$$

where

$$R_S(b; \mu) \equiv (1 - 2b)^{1+\nu} B_S(b; \mu), \quad (C8)$$

and the first coefficients in the expansion in powers of $b$ of this quantity are known from the known coefficients $r_1$ and $r_2$. We can use a combination of truncated perturbation series and Padé approximants $[1/1]$ for $R_S(b)$, as presented in Ref. [107], and obtain

$$N_m \approx 0.575(N_f = 3) \quad \approx 0.555(N_f = 4) \quad \approx 0.533(N_f = 5). \quad (C9)$$

with the uncertainties in these values of roughly ±0.020.

In the bilocal expansion $[C5]$, the analytic part $B_S^{(\text{an})}(b; \mu)$ can be taken as a polynomial in $b$, i.e., a truncated expansion in powers of $b$. The coefficients of the latter expansion can be related with $r_j(\mu^2)$’s by equating the expansion of Eq. $[C5]$ in powers of $b$ with the expansion $[C2]$, resulting in

$$B_S^{(\text{an})}(b; \mu) = h_0 + \sum_{k=1}^{n} h_k \frac{h_k}{k! \beta_0^k}, \quad (C10a)$$

$$h_k = \frac{4}{3} r_k - \pi N_m \frac{\mu}{m_q} (2\beta_0)^k \sum_{n=0}^{\infty} \tilde{c}_n \frac{\Gamma(\nu + k + 1 - n)}{\Gamma(\nu + 1 - n)}, \quad (C10b)$$

where, by convention, $r_0 = \tilde{c}_0 = 1$. The numbers $\tilde{c}_n$ of Eqs. $[C4]$, which enter the sum in Eq. $[C10b]$, are known only up to $n = 3$, because, in $\overline{\text{MS}}$, only $c_k$ up to $k = 4$ are reasonably known (c_4 approximately, as mentioned). For $N_f = 3$, these values are: $\tilde{c}_1 = -0.1638$, $\tilde{c}_2 = 0.2372$, $\tilde{c}_3 = -0.1205$ (and $\nu = 0.3951$). For $N_f = 4$, they are: $\tilde{c}_1 = -0.1054$, $\tilde{c}_2 = 0.2372$, $\tilde{c}_3 = -0.1205$, $\tilde{c}_4 = 0.0905$ (and $\nu = 0.3951$). For $N_f = 5$, they are: $\tilde{c}_1 = -0.1054$, $\tilde{c}_2 = 0.2372$, $\tilde{c}_3 = -0.1205$, $\tilde{c}_4 = 0.0905$, $\tilde{c}_5 = -0.0705$ (and $\nu = 0.3951$).
We used for the $\bar c_2 = 0.2736$, $\bar c_3 = -0.1610$ (and $\nu = 0.3696$). And for $N_f = 5$ they are: $\bar c_1 = 0.0238$, $\bar c_2 = 0.3265$, $\bar c_3 = -0.2681$ (and $\nu = 0.3289$). Therefore, the sums in (C10b) are truncated at $n = 3$.

Theoretically, the pole closest to the origin in $B_S^{(an.)}(b; \mu)$ is at $b = -1$, at least in the large-$\beta_0$ approximation.\textsuperscript{22} Nonetheless, there is a possibility that at two-loop order the kinetic term contributes to an IR renormalon at $b = -1$. This gives us

\[
\bar h_3^{(m)}(\bar m_q^2) = -25.18(N_f = 3), \ -28.28(N_f = 4), \ -35.62(N_f = 5). \tag{C11}
\]

If constructing with these values of $\bar h_3^{(m)}$ the other possible Padé approximant of index 3, namely $[1/2]_{B_S^{(an.)}}(b)$, it turns out that the nearest to origin pole of such Padé is then at $b = -1.003, -1.001, -1.008$, for $N_f = 3, 4, 5$, respectively. This indicates that the obtained values of $\bar h_3^{(m)}$, Eq. (C11), are consistent.\textsuperscript{24} Using these values, we obtain from the relation (C10b) (with the natural choice $\mu^2 = \bar m_q^2$) at $k = 3$ an estimate for $r_3$

\[
\frac{4}{3}r_3(\bar m_q^2) = \bar h_3^{(m)}(\bar m_q^2) + \pi N_m(2\bar \beta_0)^3 \sum_{n=0}^{3} \bar c_n \Gamma(\nu + 4 - n) \Gamma(\nu + 1 - n). \tag{C12}
\]

This gives us numerically the following estimates (we recall that $N_f \equiv N_\ell = 3, 4, 5$ for $c, b, t$ quark, respectively):

\[
\frac{4}{3}r_3 = 1785.9(N_f = 3), \ 1316.4(N_f = 4), \ 920.1(N_f = 5). \tag{C13}
\]

The principal origin of the uncertainties in these expressions is the uncertainty in the residue parameter $N_m$ (roughly $\pm 0.020$, i.e., less than 4%), implying an uncertainty in $r_3$ of a few percent (below 4%).

An analysis similar to this one has been performed in Ref. [76]. There, however, the term $\bar c_3$ and the coefficients $h_k^{(m)}$ were not included in the analysis. The results of Ref. [76] are: $(4/3)r_3 = 1818.6, 1346.7, 947.9.$, for $N_f = N_\ell = 3, 4, 5$, respectively. These results are by about 2-3% higher than ours [Eq. (C13)]. In another approach, applying the effective charge method (ECH) of Refs. [110] to a Euclidean analog of the quantity $m_q$, an approach using the idea of Ref. [111] extended in Ref. [81] to the mass-dependent Minkowskian quantities, the authors of Ref. [83] obtained for these coefficients the estimates $1281.05, 986.097, 719.339$, respectively. These quantities are by about 22-28% lower than ours. On the other hand, the corresponding estimates in Ref. [81] are 1544.1, 1091.0, 718.74, respectively.\textsuperscript{25}

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\textsuperscript{22} Nonetheless, there is a possibility that at two-loop order the kinetic term contributes to an IR renormalon at $b = +1$ in $B_S(b)$, cf. Ref. [105].

\textsuperscript{23} However, the $\mu$ dependence of this position is rather strong. For example, when $\mu^2$ varies by 10% around $\bar m_q^2$, the pole position in $[1/1]_{B_S^{(an.)}}$ varies between $-1.6$ and $-0.7$ in the $N_f = 3$ case, between $-1.2$ and $-0.7$ in the $N_f = 4$ case, and between $-1.26$ and $-1.00$ in the $N_f = 5$ case.

\textsuperscript{24} We used for the $\bar M$ scheme coefficient $c_4$ the estimated values [C6], with $c_4 = 123.7, 97.2, 86.2$, for $N_f = 3, 4, 5$, respectively, from Ref. [102]. Simpler Padé-based estimates of $c_4$ were obtained in Ref. [109]: $c_4 = 40, 70$ for $N_f = 4, 5$, respectively (and a large negative and uncertain value $c_4 = -850$ for $N_f = 3$). The $c_4 = 40$ value (for $N_f = 4$) in this case differs substantially from the value $c_4 = 97.2$. If we repeat for the $c_4 = 40$ value ($N_f = 4$) the same procedure described above, we obtain $\bar c_4 \approx 0.0053$ (for $c_4 = 97.2$ we got: $\bar c_4 = -0.1610$); hence the expressions of $h_k^{(m)}(\bar m_q^2)$ of Eq. (C10b) change, and the pole of $[1/1]_{B_S^{(an.)}}(b)$ becomes $b \approx -5.9$ (before: $b \approx -0.96$), not close to the theoretical pole $b = -1$. Furthermore, from the requirement that $[2/1]_{B_S^{(an.)}}(b)$ has the pole at $b = -1$ we now get $h_3^{(m)}(\bar m_q^2) = 4.10$ (before: $-28.28$), and using this value of $h_3^{(m)}$ in the Padé $[1/2]_{B_S^{(an.)}}(b)$ we obtain the pole nearest to the origin $b = 1.94$ (before: $b = -1.001$). This indicates that the estimate $c_4 = 40$ (for $N_f = 4$) is not giving results consistent with the theoretical expectations of the renormalon structure of $B_S^{(an.)}$.

\textsuperscript{25} At the time, the coefficient $r_2$ was not known, and the authors of Ref. [81] used in the estimates of $(4/3)r_3$ the analogously ECH-estimated values of $(4/3)r_2 = 124.1, 97.729, 73.616$, respectively (the exact values are 116.30, 94.21, 73.43).
Appendix D: Variation of pQCD coupling with scales and schemes

In this appendix we give the relation between \( a_0 \equiv a_{pt}(Q_0^2; c_1^{(0)}, c_3^{(0)}, \ldots) \) and \( a \equiv a_{pt}(Q^2; c_2, c_3, \ldots) \), where the latter is expressed as power expansion of the former (cf. Appendix A of Ref. [112] for details)

\[
a = a_0 + a_0^2(-x) + a_0^3(x^2 - c_1 x + \delta c_2) + a_0^4 \left( -x^3 + \frac{5}{2} c_1 x^2 - c_2^{(0)} x - 3x \delta c_2 + \frac{1}{2} \delta c_3 \right) + a_0^5 \left[ x^4 - \frac{13}{3} c_1 x^3 + \left( \frac{3}{2} c_1^2 + 3c_2^{(0)} + 6\delta c_2 \right) x^2 \right. \\
\left. + \left( -c_3^{(0)} - 3c_1 \delta c_2 - 2\delta c_3 \right) x + \left( \frac{1}{3} c_2^{(0)} \delta c_2 + \frac{5}{6} (\delta c_2)^2 - \frac{1}{6} c_1 \delta c_3 + \frac{1}{3} \delta c_4 \right) \right] + \mathcal{O}(a_0^6), \tag{D1}
\]

where we denote

\[
a \equiv a_{pt}(Q^2; c_2, c_3, \ldots), \quad a_0 \equiv a_{pt}(Q_0^2; c_1^{(0)}, c_3^{(0)}, \ldots), \tag{D2a}
\]

\[
x \equiv \beta_0 \ln \frac{Q^2}{Q_0^2}, \quad \delta c_k \equiv c_k - c_k^{(0)}. \tag{D2b}
\]

For the purposes of our paper, it is sufficient to consider in the above relation \( D1 \) terms up to (including) terms \( \sim a_0^3 \).

The three-loop threshold connection of \( a_{pt} \) in the \( \overline{\text{MS}} \) scheme at the threshold scale \( \mu_{thr}^2 = (K \bar{m}_c)^2 \) (where \( K \sim 2 \)) can be written as the following relation between \( a_{pt}(\mu_{thr}^2 + 0; N_f = 4) \equiv a_+ \) and \( a_{pt}(\mu_{thr}^2 - 0; N_f = 3) \equiv a_- \):

\[
a_+ = a_- \left[ 1 + x_1 a_- + x_2 a_-^2 + x_3 a_-^3 + \mathcal{O}(a_-^4) \right], \tag{D3}
\]

where

\[
x_1 = -k_1, \quad x_2 = -k_2 + 2k_1^2, \quad x_3 = -k_3 + 5k_1 k_2 - 5k_1^3, \tag{D4}
\]

and the coefficients \( k_j \) were calculated in Ref. [70]

\[
k_1 = -\frac{1}{6} \ell_h, \quad k_2 = \frac{1}{36} \ell_h^2 - \frac{19}{24} \ell_h + \frac{11}{72}, \quad k_3 = \frac{1}{216} \ell_h^2 - \frac{131}{576} \ell_h^3 - \frac{(6793 + 281N_\ell)}{1728} \ell_h + \left( \frac{-82043}{27648} \zeta(3) + \frac{564731}{124416} \right) \frac{2633}{31104} N_\ell, \tag{D5}
\]

where \( \ell_h = \ln(\mu_{thr}^2/\bar{m}_c^2) = \ln K^2 \), and \( N_\ell \) in Eq. \( D5 \) is the number of light quark flavors, i.e., \( N_\ell = 3 \) in the considered case of transition from \( N_f = 4 \) to \( N_f = 3 \).

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