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The b quark low-scale running mass from Υ sum rules

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Abstract

The b quark low-scale running mass $m_{\rm kin}$ is determined from an analysis of the Υ sum rules in the next-to-next-to-leading order (NNLO). It is demonstrated that using this mass one can significantly improve the convergence of the perturbation series for the spectral density moments. We obtain $m_{\rm kin}(1{\rm GeV}) = 4.56 \pm 0.06$ GeV. Using this result we derive the value of the $\overline{MS}$ mass $\bar{m}$: $\bar{m}(\bar{m}) = 4.20 \pm 0.1$ GeV. Contrary to the low-scale running mass, the pole mass of the b quark cannot be reliably determined from the sum rules. As a byproduct of our study we find the NNLO analytical expression for the cross section $e^+e^- \to Q\bar{Q}$ of the quark antiquark pair production in the threshold region, as well as the energy levels and the wave functions at the origin for the $^1S_3$ bound states of $Q\bar{Q}$.

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I. INTRODUCTION

The value of the bottom quark mass is an essential ingredient of the theoretical description of b–hadrons. Among various applications, probably the most important one at present is the determination of the Cabibbo-Kobayashi-Maskawa matrix elements from B-decays. Determination of the b quark mass is based on the sum rules for the Υ mesons, proposed about 20 years ago [1,2]. In the past several years, the sum rule analysis has been undertaken

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several times by different authors. In particular, in the paper [3] a very high accuracy of the b quark pole mass was quoted. The next attempt to extract the precise value of the b quark pole mass from the sum rules was undertaken by Jamin and Pich in [4]. Their result differed from that of Ref. [3]. The origin of the discrepancy between these two results, as well as the flaws in both derivations, were pointed out by Kühn *et al.* [5], who also determined the b quark mass. Two most recent papers on the subject [6,7] were devoted to an improvement of the theoretical accuracy of the mass determination and to a more realistic estimate of the theoretical error.

In parallel to these developments, it became more and more clear in the past years that the concept of the pole mass of a heavy quark is not a good one due to the intrinsic ambiguity of the order of $\Lambda_{\rm QCD}$ in its numerical value [9,10]. In contrast to this observation, all previous analyses were aimed at determining the pole mass of the b quark from the sum rules. We note in this respect that *practical* problems in attempts to use the pole mass in heavy quark physics are well appreciated; one of the vivid examples is provided by the calculation of the inclusive semileptonic decay widths of the B mesons (see [11] for a review). In response to this problem, it was pointed out how the "proper" quark mass relevant for non–relativistic problems can be defined [12]. In this paper we try to determine this properly defined mass from the sum rules.

For the theoretical analysis the moments of the photon polarization operator are used. These moments can be computed analytically and compared to the experimental ones. The moments of the photon vacuum polarization function are defined through the dispersion integral:

$$\mathcal{M}_n = \frac{12\pi^2 M_1^{2n}}{n!}\frac{\mathrm{d}^n}{\mathrm{d}s^n}\Pi(s)|_{s=0} = \frac{M_1^{2n}}{Q_b^2}\int\limits_0^\infty \frac{R(s)\mathrm{d}s}{s^{n+1}}, \tag{1}$$

where $R(s)$ is

$$R(s) = \frac{\sigma(e^+e^- \to b\bar{b})}{\sigma_p}, \qquad \sigma_p = \frac{4\pi\alpha^2_{\rm QED}(m_b)}{3s}. \tag{2}$$

We defined the moments to be dimensionless by multiplying them by the mass M_1 of the first Υ resonance in a suitable power. Also, $Q_b = -1/3$ is the electric charge of the b quark in units of the positron charge.

The moments $\mathcal{M}_n$ can be calculated using experimental input for $R(s)$. One gets:

$$\mathcal{M}_n^{\rm exp} = \frac{M_1^{2n}}{Q_b^2}\left(\frac{9\pi}{1.07\alpha^2_{\rm QED}}\sum_k^6 \frac{\Gamma_k}{M_k^{2n+1}} + \int\limits_{s_0}^\infty \frac{R_c(s)\mathrm{d}s}{s^{n+1}}\right), \tag{3}$$

where M_k and Γ_k are the masses and the electronic decay widths of the first six Υ resonances and $\alpha^2_{\rm QED}(m_b) = 1.07\alpha^2_{\rm QED}$ is used. The $R_c(s)$ describes the experimental spectral density, associated with the energy region above the open $B\bar{B}$ threshold; it is rather poorly known. The necessity to suppress the contribution of this region is one of the reasons for using as high values of n as possible.

On the other hand, the same moments can be calculated theoretically, using the Operator Product Expansion (OPE) for the photon polarization function. The first non–perturbative correction to the moments is associated with the gluon condensate [1,2]. It was shown that this contribution grows with n; however, for $n \leq 20$, the non-perturbative contribution to the moments was estimated to be less than one per cent [2,3]. Given exponential sensitivity of the moments to the value of the b quark mass, the influence of the non–perturbative corrections is clearly minor and can be neglected. Therefore, the whole analysis for $n \sim 10$ reduces to a careful treatment of the perturbative effects in $R(s)$. However, the perturbative treatment is not simple, since for large values of n the dominant contribution to the perturbative moments comes from the threshold energy region. The relative velocity of the $b\bar{b}$ system there is of the order of α_s. In this case, the theoretical spectral density can be calculated in the framework of the non–relativistic QCD, which means a simultaneous expansion of the spectral density in α_s and in the relative velocity β of the quark antiquark pair. As is well known, the standard perturbation theory is not adequate in the threshold region and the leading order approximation is the solution of the Coulomb problem, which resums all corrections of the form $(\alpha_s/\beta)^k$. Going to NLO and NNLO, one calculates the spectral density $R(s)$ in the threshold region resumming all $\mathcal{O}((\alpha_s/\beta)^k \times [1; \alpha_s, \beta; \alpha_s^2, \alpha_s\beta, \beta^2])$ terms. For this purpose we use the so called direct matching procedure [13] which is described e.g. in [14,15,7]. We will not discuss all necessary details of this approach here and will merely quote the results of the calculations. On the other hand, a part of the NNLO corrections was treated numerically in [14,15]; for this reason, we present some additional theoretical results, which provide the imaginary part of the polarization operator in the threshold region in completely analytical form to NNLO.

The theoretical expression for the spectral density employed in this paper reads:

$$R(s) = \lim_{r\to 0} \mathrm{Im} \left[N_c Q_b^2 \frac{24\pi}{s} \left(1 - \frac{\mathbf{p}^2}{3m^2}\right) G(\mathbf{r}, 0) \right], \tag{4}$$

where $G(\mathbf{r}, 0)$ is the Green function of the non-relativistic Schrödinger equation

$$(H - E - i\delta) G(\mathbf{r}, \mathbf{r}_1) = \delta^{(3)}(\mathbf{r} - \mathbf{r}_1), \qquad E = \sqrt{s} - 2m. \tag{5}$$

Taken literally, Eq. (4) is ill-defined due to improper treatment of the limit $r \to 0$ within the non–relativistic approach. In what follows, we circumvent this difficulty incorporating the full QCD result and matching it with its non–relativistic counterpart.

Integrating the theoretical expression for the spectral density in Eq.(1) and equating the obtained result to the experimental moments Eq.(3) one obtains the sum rules of the form:

$$\mathcal{M}_n^{\mathrm{exp}} = \mathcal{M}_n^{\mathrm{theor}}, \tag{6}$$

which give the numerical value for the b quark mass, potentially with a small uncertainty.

To summarize, the usual (and commonly used for the analysis) statement about theoretical calculations of the large-n moments can be formulated as follows: 1) for $n \sim 10 - 20$ the OPE ensures that non–perturbative corrections are small; 2) for such n the perturbative calculation of the moments requires the resummation of the Coulomb enhanced terms $\mathcal{O}(\alpha_s\sqrt{n})$. This is achieved by calculating the spectral density $R(s)$ in the threshold region which requires a resummation of the $\mathcal{O}((\alpha_s/\beta)^k) \times [1; \alpha_s, \beta; \alpha_s^2, \alpha_s\beta, \beta^2])$ terms for the NNLO accuracy. It is often assumed implicitly, that this picture is correct independently of all other parameters entering the sum rules analysis. We do not believe that this is the case. In particular, for the first point to be correct, it is crucial that one does not attempt to extract the *pole* mass of the heavy quark from the sum rules.

When this paper was prepared for publication, two other papers on this subject appeared [6,7] where the NNLO analysis of the Υ sum rules has been performed. The aim of both papers was to extract the pole mass of the b quark. In our approach to the same problem we treat the so called low energy running mass as a quantity which can be determined within the sum rule analysis; the pole mass of the b quark is used at the intermediate stages of the calculation only.

Let us present some heuristic arguments in favor of this approach. It is known that the pole mass of the quark cannot be defined when non–perturbative effects are addressed [9,10]. It is also believed that the bad behavior of the perturbation series in the relation, say between the pole mass and the $\overline{MS}$ mass, signals this. The consequence of these facts is that there is an irreducible ambiguity of the order of $\Lambda_{\rm QCD}$ in the numerical value of the pole mass. If then the pole mass of the quark is used in the sum rules analysis, its infrared sensitivity leads to new infrared effects, which have no counterpart in the standard OPE [8]. In particular, they are not described by the gluon condensate [11].

On the other hand, one can realize, that this is an artifact of the adopted procedure and the easiest way out of this problem is to abandon determination of the pole mass from the sum rule analysis. Therefore, we use the pole mass only as a tool to write the expression for the non–relativistic Hamiltonian; however, we do not treat the pole mass as a fixed number and recalculate it consistently, order by order in perturbation theory.

Instead of the pole mass, one should determine some "proper" mass, which does not suffer from a numerical ambiguity due to contributions of the soft momenta region. Such proper masses are known – one of the most familiar in this respect is the $\overline{MS}$ mass. This will not be our choice, however.

Elementary physical considerations suggest that the threshold problems are the low–scale problems, in principle. The typical scale is $\mu \sim m/\sqrt{n} \sim 1-2$ GeV for $n \sim 10$. A useful and reliable mass should therefore be normalized at such low scale $\mu \ll m$. On the other hand, in order to suppress the contribution of the infra-red region, the inequality $\Lambda_{\rm QCD} \ll \mu$ should be respected. The use of such low-scale running masses in various aspects of heavy quark physics was repeatedly advocated in the last years (for a detailed discussion and further references see [11]).

The low-scale running mass cannot be defined uniquely, because the only purpose of such definition is to remove the uncontrollable contribution of the soft momenta region which affects the pole mass. In this paper, we will work with the so called kinetic mass suggested in [12].

The relation between the pole and the kinetic masses is known to second order in α_s [16]:

$$m_{\rm pole} = m_{\rm kin}(\mu_Q) + [\Lambda(\mu_Q)]_{\rm pert} + \frac{1}{2m_{\rm kin}(\mu_Q)}\left[\mu_\pi^2(\mu_Q)\right]_{\rm pert}, \tag{7}$$

where

$$[\Lambda(\mu)]_{\rm pert} = \frac{4}{3}C_F\mu\frac{\alpha_s(\mu_1)}{\pi}\left\{1+\frac{\alpha_s}{\pi}\left[\left(\frac{4}{3}-\frac{1}{2}\ln\frac{2\mu}{\mu_1}\right)\beta_0 - C_A\left(\frac{\pi^2}{6}-\frac{13}{12}\right)\right]\right\},$$

$$\left[\mu_\pi^2(\mu)\right]_{\rm pert} = C_F\mu^2\frac{\alpha_s(\mu_1)}{\pi}\left\{1+\frac{\alpha_s}{\pi}\left[\left(\frac{13}{12}-\frac{1}{2}\ln\frac{2\mu}{\mu_1}\right)\beta_0 - C_A\left(\frac{\pi^2}{6}-\frac{13}{12}\right)\right]\right\}.$$

For the rest of this paper, α_s denotes the strong coupling constant in the $\overline{MS}$ scheme. Also, we choose μ_Q to be equal to 1 GeV, which seems to be a reasonable choice for the problem at hand. Then the ratio μ_Q/m is of the order of α_s and this gives the counting rule for the contributions to the mass which should be accounted for when one goes from one order of perturbation theory to the other. For example, to obtain the LO result we consider the pure Coulomb potential without any corrections in the non–relativistic Hamiltonian for heavy quark antiquark pair. Correspondingly, the LO relation between the pole and the kinetic masses is:

$$m_{\rm pole} = m_{\rm kin}(\mu_Q) + \frac{4}{3}C_F\frac{\alpha_s}{\pi}\mu_Q.$$

The NLO and the NNLO corrections to this expression are added in accordance with the above counting rule. Also, for our treatment, we use the same normalization scale μ_1 for the strong coupling constant in the expression for the mass, as is used in the non–relativistic Hamiltonian. This scale is called $\mu_{\rm soft}$ in the rest of the paper.

We would like to note that, according to the above counting rules, it would be necessary to know the term $\alpha_s^3\mu_Q$ in the relation between the pole mass and the kinetic mass. This term is not known at present. The BLM-type estimate [17] of this term is however available and can be extracted from [16]. Explicitly, the necessary term reads:

$$\delta\left[\Lambda(\mu)\right]_{\rm pert} = \frac{4}{3}C_F\mu\left(\frac{\alpha_s(\mu_1)}{\pi}\right)^3\left[\frac{\beta_0^2}{4}\left(\ln^2\left(\frac{\mu}{\mu_1 e}\right)+1\right) - \left(\frac{\beta_1}{8}+d_1\beta_0\right)\ln\left(\frac{\mu}{\mu_1 e}\right)+d_2\right], \quad (8)$$

where β_0 and β_1 are given in the next Section and $d_{1,2}$ read:

$$d_1 = \frac{\beta_0}{2}\left(\frac{5}{3}-\ln 2\right) - C_A\left(\frac{\pi^2}{6}-\frac{13}{12}\right),$$
$$d_2 = \left(\frac{\beta_0}{2}\right)^2\left[\left(\frac{5}{3}-\ln 2\right)^2 - \left(\frac{\pi^2}{6}-\frac{31}{36}\right)\right]. \quad (9)$$

In the numerical analysis of the last Section, we check the sensitivity of our results to the possible modification of the d_2 term due to additional terms which are not accounted for in the BLM approximation. We find, that our final result for the kinetic mass is rather insensitive to it.

As the result of our analysis, we find that the perturbation theory for the pole mass is not applicable: typically, the NNLO corrections to the pole mass exceed the NLO ones and the dependence of the result on the choice of the scale of the strong coupling constant is very strong. These unwelcome features, therefore, do not permit a reliable determination of the b quark pole mass from the sum rules, with a trustworthy estimate of the theoretical uncertainty.

On the contrary, the situation with the low-scale running mass looks more healthy: the perturbation series seem to be sign alternating and the dependence on the normalization scale for the coupling constant appears to be reduced, as compared to the pole mass.

The rest of the paper is organized as follows: in the next Section we discuss the framework of the calculation. In Section 3 the corrections to the Green function due to corrections to the static quark antiquark potential are derived. In Section 4 the corrections to the Green function due to relativistic corrections to the heavy quark Hamiltonian are obtained. In Section 5 we combine these results and present the NNLO expression for the theoretical spectral density $R(s)$ in the threshold region. In Section 6 the results for the energy levels and the wave functions at the origin for the ${}^1S_3$ $Q\bar{Q}$ resonances are derived. In Section 7 we present our final analysis for the sum rules and determine the low-scale mass of the b quark. Finally we present our conclusions.

II. THE FRAMEWORK OF THE CALCULATION

We first discuss a framework of our calculations and introduce all relevant notations. As we mentioned already, in order to obtain the expression for the theoretical spectral density, we have to calculate the expression for the imaginary part of the polarization operator in the threshold region. The threshold region is characterized by a small value of the quark velocity β:

$$\beta = \sqrt{1 - \frac{4m^2}{s}} \ll 1. \tag{10}$$

Here and below m is the pole mass. The pole mass enters the usual perturbative expansion in quantum mechanics for the nonrelativistic quarks. Later we will extract the low-scale running mass from the pole one.

Dynamics of slow moving quark antiquark pair is governed by the non–relativistic Hamiltonian:

$$\begin{aligned}
H &= H_0 + V_1(r) + U(\mathbf{p}, \mathbf{r}), \\
H_0 &= \frac{\mathbf{p}^2}{m} - \frac{C_F a_s}{r}, \\
V_1(r) &= -\frac{C_F a_s^2}{4\pi r}\Bigg[2\beta_0 \ln(2\mu' r) + a_1 \\
&+ \left(\frac{a_s}{4\pi}\right)\left(\beta_0^2\left(4\ln^2(\mu' r) + \frac{\pi^2}{3}\right) + 2(\beta_1 + 2\beta_0 a_1)\ln(\mu' r) + a_2\right)\Bigg], \\
U(\mathbf{p}, \mathbf{r}) &= -\frac{\mathbf{p}^4}{4m^3} + \frac{\pi C_F a_s}{m^2}\delta^3(\mathbf{r}) - \frac{C_F a_s}{2m^2 r}\left(\mathbf{p}^2 + \frac{\mathbf{r}(\mathbf{r}\mathbf{p})\mathbf{p}}{r^2}\right) \\
&+ \frac{3C_F a_s}{2m^2 r^3}\mathbf{S}\mathbf{L} - \frac{C_F a_s}{2m^2}\left(\frac{\mathbf{S}^2}{r^3} - 3\frac{(\mathbf{S}\mathbf{r})^2}{r^5} - \frac{4\pi}{3}(2\mathbf{S}^2 - 3)\delta(\mathbf{r})\right) - \frac{C_A C_F a_s^2}{2mr^2}.
\end{aligned} \tag{11}$$

In the above equations, the strong coupling constant is evaluated at the scale μ_{soft}:

$$a_s = \alpha_s(\mu_{\text{soft}}). \tag{12}$$

The scale μ' equals to μe^{γ_E}.

The operator $U(\mathbf{p},\mathbf{r})$ is the QCD generalization of the standard Breit potential [18]. The last term in the expression for the operator $U(\mathbf{p},\mathbf{r})$ is the non–Abelian contribution, originating from a correction to the Coulomb exchange, caused by a transverse gluon [19]. The potential $V_1(r)$ represents a deviation of the static QCD potential from the Coulomb one. It was calculated to order α_s^2 in [20] and to order α_s^3 in [21]. The coefficients there read explicitly:

$$
\begin{aligned}
\beta_0 &= \frac{11}{3}C_A - \frac{4}{3}N_L T_R, \\
\beta_1 &= \frac{34}{3}C_A^2 - \frac{20}{3}C_A T_R N_L - 4C_F T_R N_L, \\
a_1 &= \frac{31}{9}C_A - \frac{20}{9}T_R N_L, \\
a_2 &= \left(\frac{4343}{162} + 6\pi^2 - \frac{\pi^4}{4} + \frac{22}{3}\zeta_3\right) C_A^2 - \\
&\left(\frac{1798}{81} + \frac{56}{3}\zeta_3\right) C_A T_R N_L - \left(\frac{55}{3} - 16\zeta_3\right) C_F T_R N_L + \left(\frac{20}{9}T_R N_L\right)^2 .
\end{aligned} \tag{13}
$$

The $SU(3)$ color factors are $C_A = 3, C_F = 4/3, T_R = 1/2$. $N_L = 4$ is the number of quarks whose masses have been neglected.

Given the Hamiltonian H, one can find the Green function of the Schrödinger equation:

$$
(H - E - i\delta)G(\mathbf{r},\mathbf{r}_1) = \delta^{(3)}(\mathbf{r}-\mathbf{r}_1), \qquad E = \sqrt{s} - 2m. \tag{14}
$$

Once the Green function is found, the non–relativistic cross section for the $Q\bar{Q}$ pair production in e^+e^- annihilation is obtained using Eq.(4).

Treating the corrections to the Green function in the perturbation theory, one can consider the corrections due to $V_1(r)$ and $U(\mathbf{p},\mathbf{r})$ separately. The corrections to the Green function due to $U(\mathbf{p},\mathbf{r})$ were recently calculated in [14,15]. These corrections are not simple conceptually, because they deliver divergent contributions to the Green function at the origin. The divergences are removed by matching the result of the calculations in quantum mechanics to the result of the full QCD calculation [22]. Technically, however, the calculation of the correction caused by $U(\mathbf{p},\mathbf{r})$ is very simple and can be performed algebraically (see [15]). On the other hand, the corrections to the imaginary part of the Green function due to the $V_1(r)$ perturbation can be calculated within the quantum mechanics and for this reason these corrections are rather simple conceptually. However, they provide the most challenging part of the whole calculation from the technical viewpoint. For this reason, the calculation of the corrections to the imaginary part of the Green function due to the $V_1(r)$ perturbation is discussed below in some detail.

III. CORRECTIONS TO THE GREEN FUNCTION DUE TO $V_1(R)$

A. The Coulomb Green function

In this section we collect useful formulas for the Coulomb Green function. A convenient expression for the S-wave Coulomb Green function can be found in [23]:

$$G(r,r_1) = \frac{-ime^{ik(r+r_1)}}{4\pi\sqrt{rr_1}} \int\limits_0^\infty \frac{\mathrm{d}t}{\sqrt{t(t+1)}} \left(\frac{1+t}{t}\right)^{i\nu} e^{2ik(r+r_1)t} J_1(4k\sqrt{rr_1}\sqrt{t(t+1)}), \tag{15}$$

In the above expression, $\nu = C_F\alpha_s/(2\beta)$ and $k = m\beta$.

Using this representation, one easily obtains the expression for $G(r,0)$:

$$G(r,0) = \frac{-imk}{2\pi} e^{ikr} \int\limits_0^\infty \mathrm{d}t \left(\frac{1+t}{t}\right)^{i\nu} e^{2ikrt}. \tag{16}$$

From the expression for the cross section (cf. Eq. (4)), it is clear, that one is interested in the behavior of the Coulomb Green function for small r. For small r, the Green function diverges like $1/r$; the principal divergence is related to the behavior of the free ($\alpha_s = 0$) Green function:

$$G^{(0)}(r,0) = \frac{m}{4\pi r} e^{ikr}. \tag{17}$$

B. Generating function

To calculate corrections to the Coulomb Green function at the origin caused by the $V_1(r)$ perturbation, it is convenient to introduce a generating function $g(\sigma)$:

$$g(\sigma) = \int d^3\mathbf{r}\; G^2(r,0) \frac{(2\mu r)^\sigma}{r}. \tag{18}$$

Once this function is found, one easily obtains a correction to the Green function at the origin caused by the $V_1(r)$ term in the potential. For further calculations, it will be convenient to separate the generating function into two terms:

$$g(\sigma) = g_{\rm free}(\sigma) + g_1(\sigma), \tag{19}$$

where

$$\begin{aligned} g_{\rm free}(\sigma) &= \int \mathrm{d}^3\mathbf{r}\; G_0^2(r,0) \frac{(2\mu r)^\sigma}{r}, \\ g_1(\sigma) &= \int \mathrm{d}^3\mathbf{r}\; \left\{G^2(r,0) - G_0^2(r,0)\right\} \frac{(2\mu r)^\sigma}{r}. \end{aligned} \tag{20}$$

In the above equations, $G_0(r,0)$ is the free Green function (cf. Eq. (17)).

It is an easy task to calculate $g_{\rm free}$. One gets:

$$g_{\rm free} = \frac{m^2}{4\pi} \left(\frac{i\mu}{k}\right)^\sigma \Gamma(\sigma). \tag{21}$$

We need further $g_1(\sigma)$. For the Coulomb Green function we use the representation from Eq. (16). Integrating then over $\mathbf{r}$ in Eq. (20), one gets:

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \Gamma(2+\sigma)\int\limits_0^\infty dtds\left[\left(\frac{1+t}{t}\right)^{i\nu}\left(\frac{1+s}{s}\right)^{i\nu} - 1\right](1+t+s)^{-2-\sigma}. \qquad (22)$$

To proceed further, it is convenient to introduce new integration variables,

$$\tau = \frac{t}{1+t}, \qquad \rho = \frac{s}{1+s}. \qquad (23)$$

Then one gets:

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \Gamma(2+\sigma)\int\limits_0^1 d\tau d\rho\frac{\tau^{-i\nu}\rho^{-i\nu}-1}{(1-\tau)^{-\sigma}(1-\rho)^{-\sigma}}(1-\rho\tau)^{-2-\sigma}. \qquad (24)$$

Substituting also $\eta = \rho\tau$ we arrive at:

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \Gamma(2+\sigma)\int\limits_0^1 d\eta\frac{\eta^{-i\nu}-1}{(1-\eta)^{2+\sigma}}\int\limits_\eta^1 \frac{d\tau}{\tau}(1-\tau)^\sigma\left(1-\frac{\eta}{\tau}\right)^\sigma. \qquad (25)$$

Finally, changing the variables $\tau \to \xi$ with $\xi = (1-\tau)/(1-\eta)$, we get

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \Gamma(2+\sigma)\int\limits_0^1 d\eta\frac{\eta^{-i\nu}-1}{(1-\eta)^{1-\sigma}}\int\limits_0^1 d\xi\xi^\sigma(1-\xi)^\sigma\left(1-(1-\eta)\xi\right)^{-\sigma-1}. \qquad (26)$$

The last integral is proportional to $F_{21}(1+\sigma, 1+\sigma; 2+2\sigma; 1-\eta)$ and equals to

$$\int\limits_0^1 \mathrm{d}\xi\frac{\xi^\sigma(1-\xi)^\sigma}{(1-(1-\eta)\xi)^{\sigma+1}} = \sum_{n=0}^\infty \frac{(1+\sigma)_n^2}{(n!)^2}\left[2\psi(n+1) - 2\psi(1+n+\sigma) - \ln\eta\right]\eta^n, \qquad (27)$$

where the series representation for the hypergeometric function was used. Here $(z)_n = \Gamma(z+n)/\Gamma(z)$ is the Pochhammer symbol. Integrating over η, we obtain

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \Gamma(2+\sigma)\Gamma(\sigma)\sum_{n=0}^\infty \frac{(1+\sigma)_n^2}{(n!)^2}\left[2\psi(n+1) - 2\psi(n+1+\sigma) - \partial_n\right] \times \left\{\frac{\Gamma(n+1-i\nu)}{\Gamma(n+1-i\nu+\sigma)} - \frac{\Gamma(n+1)}{\Gamma(n+1+\sigma)}\right\}, \qquad (28)$$

which can be presented in a more compact form[1]:

$$g_1(\sigma) = -\frac{m^2}{4\pi}\left(\frac{i\mu}{k}\right)^\sigma \frac{1+\sigma}{\sigma}\sum_{n=1}^\infty \partial_n\left\{\frac{\Gamma^2(n+\sigma)}{\Gamma^2(n)}\frac{\Gamma(n-i\nu)}{\Gamma(n-i\nu+\sigma)} - \frac{\Gamma(n+\sigma)}{\Gamma(n)}\right\}. \qquad (29)$$

In Eqs.(28,29) ∂_n stands for the partial derivative with respect to n. Eqs. (19,21,29) provide a necessary expression for the generating function.

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[1]We thank O. Yakovlev for pointing this to us.

C. Correction to the Green function due to $\ln^n(2\mu r)/r,\ n \le 2$ perturbation

To evaluate these corrections we will use the representation of the generating function $g(\sigma)$ given in the previous section. For the case of interest, the correction to the imaginary part of the Green function at the origin due to $\ln^n(2\mu r)/r$ perturbation is obtained as the n-th derivative of the imaginary part of the generating function with respect to σ at $\sigma \to 0$. To obtain these derivatives, we first expand the generating function up to the second order in σ:

$$g_{\rm free}(\sigma) = \frac{m^2}{4\pi}\left\{\frac{1}{\sigma} + \ln\frac{i\mu}{k} - \gamma_E + \frac{\sigma}{2}\left[\left(\ln\frac{i\mu}{k} - \gamma_E\right)^2 + \frac{\pi^2}{6}\right]\right.$$
$$\left. + \frac{\sigma^2}{6}\left[\left(\ln\frac{i\mu}{k} - \gamma_E\right)^3 + \frac{\pi^2}{2}\left(\ln\frac{i\mu}{k} - \gamma_E\right) - 2\zeta_3\right] + \ldots\right\}; \tag{30}$$

and

$$g_1(\sigma) = \frac{m^2}{4\pi}\left(g_1(0) + \sigma g_1'(0) + \frac{\sigma^2}{2} g_1''(0) + \ldots,\right) \tag{31}$$

where

$$g_1(0) = -\sum_{n=1}^{\infty} \partial_n\left(\psi(n) - \psi(n - i\nu)\right) = -\gamma_E - \partial_{i\nu} i\nu\ \psi(1 - i\nu), \tag{32}$$

$$g_1'(0) = \left(\ln\frac{i\mu}{k} + 1\right) g_1(0) + \frac{\pi^2}{6} + \frac{1}{2}\partial_{i\nu}^2 i\nu\ \psi(1 - i\nu)$$
$$-\frac{1}{2}\sum_{n=1}^{\infty} \partial_n\left[\left(\psi(n) - \psi(n - i\nu)\right)\left(3\psi(n) - \psi(n - i\nu)\right)\right], \tag{33}$$

$$g_1''(0) = 2\left(\ln\frac{i\mu}{k} + 1\right) g_1'(0) - \left\{\left(\ln\frac{i\mu}{k} + 1\right)^2 + 1\right\} g_1(0) - \frac{1}{3}\partial_{i\nu}^3 i\nu\ \psi(1 - i\nu)$$
$$-\frac{1}{3}\sum_{n=1}^{\infty} \partial_n\left\{\frac{3}{2}\left(3\psi^2(n) - 4\psi(n)\psi(n - i\nu) + \psi^2(n - i\nu)\right)'\right.$$
$$\left. + 7\psi^3(n) - 12\psi^2(n)\psi(n - i\nu) + 6\psi(n)\psi^2(n - i\nu) - \psi^3(n - i\nu)\right\}. \tag{34}$$

Using these expressions, we easily find the corrections to the imaginary part of the Green function at the origin, caused by $\ln^n(2\mu r)/r$ perturbations. In the formulas below we disregard the $1/\sigma$ pole which is present in the expression for $g_{\rm free}$ since it does not contribute to the imaginary part. We obtain explicitly:

$$\delta G_L(\mu) = -\int {\rm d}^3\mathbf{r} G(r,0)^2 \frac{\ln(2\mu r)}{r} = \frac{-m^2}{4\pi}\left\{\frac{1}{2}\left[\left(\ln\frac{i\mu}{k} - \gamma_E\right)^2 + \frac{\pi^2}{6}\right] + g_1'(0)\right\}. \tag{35}$$

In a similar manner one obtains the correction due to $\ln^2(2\mu r)/r$ perturbation:

$$\delta G_{L2}(\mu) = -\int {\rm d}^3\mathbf{r} G(r,0)^2 \frac{\ln^2(2\mu r)}{r} =$$
$$\frac{-m^2}{4\pi}\left\{\frac{1}{3}\left[\left(\ln\frac{i\mu}{k} - \gamma_E\right)^3 + \frac{\pi^2}{2}\left(\ln\frac{i\mu}{k} - \gamma_E\right) - 2\zeta_3\right] + g_1''(0)\right\}. \tag{36}$$

D. The second iteration of the logarithmic perturbation

The leading term of the static potential $V_1(r)$ provides an $\mathcal{O}(\alpha_s)$ correction. Therefore, one should calculate the second order correction induced by the perturbation $\ln(2\mu r)/r$. Such calculation is described below.

Explicitly, we have to calculate:

$$\delta G^{(2)}(\mu) = \int \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{r}_1 G(r,0)V(r)G(r,r_1)V(r_1)G(r_1,0), \qquad V(r) = \ln(2\mu r)/r. \tag{37}$$

For this purpose we use the representation for the Green function $G(r,r_1)$, given in Eq. (15). We define:

$$G_1(\sigma,\sigma_1) = \left(\frac{i\mu}{k}\right)^{\sigma+\sigma_1} \frac{1}{\Gamma(-\sigma)\Gamma(-\sigma_1)} \int\limits_0^\infty \frac{\mathrm{d}\tau \mathrm{d}\tau_1}{\tau^{1+\sigma}\tau_1^{1+\sigma_1}} F(\tau,\tau_1), \tag{38}$$

where

$$F(\tau,\tau_1) = \int \mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{r}_1 G(r,0)\frac{e^{2ikr\tau}}{r}G(r,r_1)\frac{e^{2ikr_1\tau_1}}{r_1}G(r_1,0). \tag{39}$$

Then

$$\delta G^{(2)} = \frac{\partial^2}{\partial_\sigma \partial_{\sigma_1}} G_1(\sigma,\sigma_1)|_{\sigma=0,\sigma_1=0}. \tag{40}$$

Using Eqs. (15,16) for the Green functions, and performing the integrations over r, r_1 and the variable t which enters the integral representation of the $G(r,r_1)$ function, we arrive at the following result:

$$F(\tau,\tau_1) = \frac{im^3}{8\pi k(1-i\nu)} F_1(\tau,\tau_1), \tag{41}$$

$$F_1(\tau,\tau_1) = \int\limits_0^1 \frac{\mathrm{d}u\, \mathrm{d}v}{\Delta^2\Delta_1^2} \left(\frac{1+u}{u}\right)^{i\nu} \left(\frac{1+v}{v}\right)^{i\nu} F_{21}\left(2, 1-i\nu; 2-i\nu; \frac{(\Delta-1)(\Delta_1-1)}{\Delta\Delta_1}\right), \tag{42}$$

where

$$\Delta = 1+u+\tau, \qquad \Delta_1 = 1+v+\tau_1, \tag{43}$$

and $F_{21}(a,b;c;z)$ is the Gauss hypergeometric function.

The function $G_1(\sigma,\sigma_1)$ can be written as

$$G_1(\sigma,\sigma_1) = \left(\frac{i\mu}{k}\right)^{\sigma+\sigma_1} \frac{im^3}{8\pi k(1-i\nu)} W(\sigma,\sigma_1), \tag{44}$$

where

$$W(\sigma,\sigma_1) = \frac{1}{\Gamma(-\sigma)\Gamma(-\sigma_1)} \int\limits_0^\infty \frac{d\tau\; d\tau_1}{\tau^{1+\sigma}\tau^{1+\sigma_1}} F_1(\tau,\tau_1). \tag{45}$$

For further calculation, it is convenient to define new variables

$$u \to u_1 = u - \tau; \qquad v \to v_1 = v - \tau_1$$

and integrate over τ and τ_1. Performing another variable transformation,

$$u_1 \to x = \frac{u_1}{1+u_1} \qquad v_1 \to y = \frac{v_1}{1+v_1},$$

we finally get:

$$W(\sigma,\sigma_1) = \frac{\Gamma(1-i\nu)^2}{\Gamma(1-i\nu-\sigma)\Gamma(1-i\nu-\sigma_1)} \int\limits_0^1 dx\; dy \left(\frac{x}{1-x}\right)^{-\sigma} \left(\frac{y}{1-y}\right)^{-\sigma_1} (xy)^{-i\nu}$$
$$F_{21}(-i\nu,-\sigma;1-i\nu-\sigma;x) F_{21}(-i\nu,-\sigma_1;1-i\nu-\sigma_1;y) F_{21}(2,1-i\nu;2-i\nu;xy).$$

One notes that if the last hypergeometric function in the above equation is expanded in Taylor series in xy, integrations over x and y factorize. These series would, however, diverge for $xy=1$. Nevertheless, upon integration over x and y, one gets a series which converges as $1/n^2$. We conclude therefore, that this operation is legitimate. We write $W(\sigma,\sigma_1)$ in a factorized form:

$$W(\sigma,\sigma_1) = \frac{\Gamma(1-i\nu)^2(1-i\nu)}{\Gamma(1-i\nu-\sigma)\Gamma(1-i\nu-\sigma_1)} \sum_{n=1}^{\infty} \frac{n}{n-i\nu} T(n,\sigma) T(n,\sigma_1), \tag{46}$$

where

$$T(n,\sigma) = \int\limits_0^1 dx x^{n-1-i\nu} \left(\frac{x}{x-1}\right)^{-\sigma} F_{21}(-i\nu,-\sigma;1-i\nu-\sigma;x). \tag{47}$$

According to Eq.(40), one needs an expansion of $T(n,\sigma)$ in σ up to the first power. This can be easily done by expanding the hypergeometric function in Taylor series in Eq.(47), evaluating resulting integrals, extracting the limit $\sigma \to 0$ and then resumming the resulting series. We obtain:

$$T(n,\sigma) = \frac{1}{n-i\nu} - \sigma T_1(n), \tag{48}$$

where

$$T_1(n) = \frac{2\gamma}{n-i\nu} + \frac{\psi(1-i\nu)}{n} + \frac{\psi(n-i\nu)(n+i\nu)}{n(n-i\nu)} + \frac{i\nu}{n(n-i\nu)^2}. \tag{49}$$

With this result, we obtain the series representation for the function $W(\sigma,\sigma_1)$ with the required accuracy in σ,σ_1. Upon differentiation over σ and σ_1 at $\sigma=\sigma_1=0$ we get the correction to the Green function $\delta G^{(2)}$:

$$\delta G^{(2)}(\mu) = \frac{im^3}{8\pi k} \left\{ \sum_{n=1}^{\infty} \frac{n}{n-i\nu} \left(\frac{\ln\left(\frac{i\mu}{k}\right) + \psi(1-i\nu)}{n-i\nu} - T_1(n) \right)^2 \right\}.$$

IV. CORRECTIONS TO THE GREEN FUNCTION DUE TO THE $U(\mathbf{p},\mathbf{r})$ PERTURBATION

We now briefly discuss corrections to the Green function at the origin caused by the operator $U(\mathbf{p},\mathbf{r})$ from Eq.(11). This correction is obtained as

$$\delta G^U = -\int \mathrm{d}^3\mathbf{r} G(r,0)\; U(\mathbf{p},\mathbf{r})\; G(r,0). \tag{50}$$

As long as we are interested in the $Q\bar{Q}$ pairs, produced in the triplet S–states, only the corresponding projection of the operator $U(\mathbf{p},\mathbf{r})$ should be considered. Substituting $\mathbf{S}^2 = 1$ and $\mathbf{SL} = 0$ in Eq.(11), it is easy to get that $U(\mathbf{p},\mathbf{r})$ can be presented in the following form:

$$U(\mathbf{p},\mathbf{r}) = -\frac{\mathbf{p}^4}{4m^3} + \frac{11\pi a_s C_F}{3m^2}\delta^{(3)}(\mathbf{r}) - \frac{C_F a_s}{2m^2}\left\{\frac{1}{r},\mathbf{p}^2\right\} - \frac{C_A C_F a_s^2}{2mr^2}. \tag{51}$$

At this stage, it is advantageous to express this operator in terms of the zeroth order Hamiltonian H_0 in order to apply the equation of motion for the Green function $G(r,0)$:

$$(H_0 - E)G(r,0) = \delta^{(3)}(\mathbf{r}). \tag{52}$$

This is most easily done using the following commutation relations:

$$[H_0, ip_r] = \frac{4\pi\delta^{(3)}(\mathbf{r})}{m} + \frac{2\mathbf{L}^2}{mr^3} - \frac{C_F a_s}{r^2}, \tag{53}$$

$$\left\{H_0, \frac{1}{r}\right\} = \frac{2}{r}H + \frac{4\pi\delta^{(3)}(\mathbf{r})}{m} + \frac{2}{mr^2}\partial_r, \tag{54}$$

where $p_r = -i(\partial_r + 1/r)$ is the radial momentum operator. One finds that the operator $U(\mathbf{p},\mathbf{r})$ from Eq. (51) can be written as:

$$U(\mathbf{p},\mathbf{r}) = -\frac{H_0^2}{4m} - \frac{3C_F a_s}{4m}\left\{H_0, \frac{1}{r}\right\} + \frac{11C_F a_s}{12m}[H_0, ip_r] - \frac{(2C_F + 3C_A)\, C_F a_s^2}{6mr^2}. \tag{55}$$

Let us consider the first three terms of Eq. (55). Inserting them into Eq. (50) and using the equation of motion for the Green function (52), we find:

$$\begin{aligned} &-\int \mathrm{d}^3\mathbf{r} G(r',r)\left(-\frac{H_0^2}{4m} - \frac{3C_F a_s}{4m}\left\{H, \frac{1}{r}\right\} + \frac{11C_F a_s}{12m}[H, ip_r]\right) G(r,r'') \\ &= \left[\frac{E}{2m} + \frac{3C_F a_s}{2mr}\right] G(r,0) + 2ip_r G(r,0) + \int \mathrm{d}^3\mathbf{r} G(0,r)\left\{\frac{E^2}{4m} + \frac{3C_F a_s E}{2mr}\right\} G(r,0). \end{aligned} \tag{56}$$

All terms in the above equation which cannot contribute to the imaginary part of the Green function have been omitted.

Also, it is easy to recognize that the terms in Eq. (56), which still have to be integrated over $\mathbf{r}$, can be easily obtained if one redefines the eigenvalue and the coupling constant of the lowest order Hamiltonian H_0:

$$H_0 \to \mathcal{H} = \frac{\mathbf{p}^2}{m} - \frac{C_F a_s}{r}\left(1+\frac{3E}{2m}\right); \qquad E \to \mathcal{E} = E + \frac{E^2}{4m} = \frac{p_0^2}{m} = \frac{m\beta^2}{1-\beta^2}. \tag{57}$$

The new Hamiltonian $\mathcal{H}$ is still of the Coulomb form and, therefore, the solution for the Coulomb Green function presented in the previous section can be used.

Therefore, we conclude, that the only non–trivial calculation required here is the correction to the Green function at the origin caused by the $1/r^2$ perturbation, which is explicitly given by the last term in Eq. (55). We refer the reader to the paper [15] where the details of the calculation are discussed.

V. COMPLETE RESULT AND MATCHING

We now combine the results of the above calculations and write the final result in the form:

$$R(s) = \mathcal{K}(\mu_{\rm hard}, \mu_{\rm fact})\ (R_1(s) + R_2(s)), \tag{58}$$

$$\begin{aligned} R_1(s) &= \frac{3}{2} N_c Q_b^2 C_F a_s {\rm Im}\left\{ H(C_F a_s, \beta)\left[1 + C_F a_s^2\left(\frac{C_F}{3}+\frac{C_A}{2}\right) H(C_F a_s,\beta)\right]\right\}, \\ R_2(s) &= \frac{6\pi C_F}{m^2} N_c Q_b^2 {\rm Im}\Bigg\{ \frac{-2a_s^2}{4\pi}\left[\beta_0 + \frac{a_s}{4\pi}(\beta_1 + 2\beta_0 a_1)\right]\delta G_L\left(\frac{\mu_a}{2}\right) - \frac{4\beta_0^2 a_s^3}{(4\pi)^2}\delta G_{L2}\left(\frac{\mu_1}{2}\right) + \\ &\quad \frac{4\beta_0^2 C_F a_s^4}{(4\pi)^2}\delta G^{(2)}\left(\frac{\mu_b}{2}\right)\Bigg\}. \end{aligned} \tag{59}$$

In the above expression, R_2 is the contribution due to the $V_1(r)$ perturbation. The scales μ_1, μ_a, μ_b there read explicitly:

$$\mu_1 = \mu_{\rm soft}\exp[\gamma_E], \qquad \mu_a = \mu_1 \exp\left[\frac{a_1 + \frac{a_s}{4\pi}(\frac{\pi^2}{3}\beta_0^2 + a_2)}{2\beta_0 + \frac{a_s}{4\pi}2(\beta_1 + 2\beta_0 a_1)}\right], \qquad \mu_b = \mu_1\exp\left[\frac{a_1}{2\beta_0}\right]. \tag{60}$$

The function $H(a,\beta)$ was first obtained in a similar context in [13] and is given by:

$$H(a,\beta) = \left(1-\frac{\beta^2}{3}\right)\left\{\frac{i\beta}{a} - (1+\beta^2)\left[\gamma_E + \ln\left(\frac{-i\beta m}{\mu_{\rm fact}}\right) + \psi\left(1 - ia\frac{1+\beta^2}{2\beta}\right)\right]\right\}. \tag{61}$$

We have absorbed all energy-independent divergent contributions to the factor $\mathcal{K}(\mu_{\rm hard}, \mu_{\rm fact})$, which is determined by matching the above result for $R(s)$ to the result of the perturbative calculations in full QCD [22] in the region $\alpha_s \ll \beta \ll 1$, where both results are supposed to be valid. One gets:

$$\mathcal{K}(\mu_{\rm hard}, \mu_{\rm fact}) = 1 + C_1 C_F\left(\frac{\alpha_s(\mu_{\rm hard})}{\pi}\right) + C_2 C_F\left(\frac{\alpha_s(\mu_{\rm hard})}{\pi}\right)^2, \tag{62}$$

$$C_1 = -4; \qquad C_2 = C_F C_2^A + C_A C_2^{NA} + T_R N_L C_2^L + T_H N_H C_2^H - C_1\frac{\beta_0}{4}\ln\left(\frac{m^2}{\mu_{\rm hard}^2}\right), \tag{63}$$

and

$$
\begin{aligned}
C_2^A &= \frac{39}{4} - \zeta_3 + \pi^2\left(\frac{4}{3}\ln 2 - \frac{35}{18}\right) + \frac{\pi^2}{3}\ln\frac{m^2}{\mu_{\rm fact}^2};\\
C_2^{NA} &= -\frac{151}{36} - \frac{13}{2}\zeta_3 + \pi^2\left(\frac{179}{72} - \frac{8}{3}\ln 2\right) + \frac{\pi^2}{2}\ln\frac{m^2}{\mu_{\rm fact}^2};\\
C_2^H &= \frac{44}{9} - \frac{4}{9}\pi^2;\\
C_2^L &= \frac{11}{9}.
\end{aligned}
\tag{64}
$$

VI. CORRECTIONS TO THE ENERGY LEVELS AND THE WAVE FUNCTIONS

It is known, that the proper expression for the Green function which is valid in the whole threshold energy region is given by the expression:

$$
G(E+i\epsilon;0,0) = \sum_n \frac{|\Psi_n|^2}{E_n - E - i\epsilon} + \int\limits_0^\infty \frac{dk}{2\pi}\frac{|\Psi_k|^2}{E_k - E - i\epsilon}. \tag{65}
$$

Here E_n and Ψ_n are the energy levels and the wave functions at the origin of the perturbative $^3S_1$ $\bar{Q}Q$ resonances, which can be calculated order by order in perturbation theory. On the other hand, when a correction to the Green function is calculated as a power series over a perturbation, the energy denominators entering the exact expression (65) are also expanded in powers of α_s. It is therefore possible to extract the corrections to the energy levels and to the wave functions of the resonances by performing the Laurent expansion around $E = E_n^{(0)}$ of the corrections to the Green function obtained in the previous sections. On one hand, these results are interesting by itself, for applications to various problems that involve perturbative calculations for bound states both in QED and QCD. On the other hand, they are used below to construct the proper theoretical expression for the large–n moments.

In the formulas below we denote:

$$
\psi_z = \psi(z),\ \psi'_z = \frac{\mathrm{d}}{\mathrm{d}z}\psi(z),\ \text{etc.}
$$

To present our results, it turns out to be useful to define a function

$$
S_i(n) = \sum_{k=1}^{n-1}\frac{\psi_k}{k^i}. \tag{66}
$$

The energy levels and the wave functions at the lowest order are given by:

$$
E_n^{(0)} = -\frac{m(C_F\alpha_s(\mu))^2}{4n^2}, \qquad |\Psi_n^{(0)}|^2 = \frac{(mC_F\alpha_s(\mu))^3}{8\pi n^3}. \tag{67}
$$

First we present an expression for the energy levels valid up to (relative) order $\mathcal{O}(\alpha_s^2)$:

$$E_n = E_n^{(0)}\Bigg\{1+\frac{\alpha_s}{\pi}\left(\beta_0+\frac{\alpha_s}{4\pi}\left(\beta_1+2\beta_0 a_1\right)\right)\left(L(\mu_a)+\psi_{n+1}\right)$$
$$+\left(\frac{\alpha_s\beta_0}{2\pi}\right)^2 2\left[\left(L(\mu_1)+\psi_{n+1}\right)^2-\psi'_{n+1}-2\frac{\psi_{n+1}+\gamma_E}{n}+\frac{\pi^2}{3}\right]$$
$$+\left(\frac{\alpha_s\beta_0}{2\pi}\right)^2\left[\left(L(\mu_b)+\psi_{n+1}-1\right)^2-1-2\psi_n^{'}-n\psi_n^{''}+\frac{2}{n}\left(\psi_{n+1}+\gamma_E\right)\right]$$
$$-\frac{(C_F\alpha_s)^2}{n}\left(\frac{11}{16n}-\frac{2}{3}-\frac{C_A}{C_F}\right)\Bigg\}, \tag{68}$$

where $\mu=\mu_{\rm soft}$,

$$L(\mu)=\ln\left(\frac{\mu n}{C_F\alpha_s m}\right)$$

and the scales μ_1,μ_a,μ_b are defined in Eq.(60). This result is in agreement with the one obtained in [24].

Using the same notations, we obtain the result for the square of the wave functions at the origin:

$$|\Psi_n|^2 = |\Psi_n^{(0)}|^2\,\mathcal{K}(\mu_{\rm hard},\mu_{\rm fact})\Bigg\{1+\left(\frac{\alpha_s}{2\pi}\right)\left(\beta_0+\frac{\alpha_s}{4\pi}\left(\beta_1+2\beta_0 a_1\right)\right)\left[3\left(L(\mu_a)+\psi_{n+1}\right)-\right.$$
$$\left.2\left(n\psi'_n+\psi_n+\gamma_E\right)-1\right]+\frac{3}{2}\left(\frac{\alpha_s\beta_0}{2\pi}\right)^2 2\left[\left(L(\mu_1)+\psi_{n+1}\right)^2-\psi'_{n+1}-2\frac{\psi_{n+1}+\gamma_E}{n}+\frac{\pi^2}{3}\right]$$
$$-2\left(\frac{\alpha_s\beta_0}{2\pi}\right)^2\left[L(\mu_1)(2n\psi'_n+2\psi_n+2\gamma_E+1)+2n\psi'_n\left(\psi_n-\gamma_E\right)+\psi_n\left(1-2\gamma_E-\frac{2}{n}\right)\right.$$
$$\left.+2nS_2(n+1)-2n\zeta_3+2\zeta_2(1+\gamma_E n)+\frac{1}{n}-2\gamma_E^2\right]$$
$$+\left(\frac{\alpha_s\beta_0}{2\pi}\right)^2\left[3L(\mu_b)^2-\frac{\left(4n^2\psi'_n-2n\psi_n+n(5+4\gamma_E)-6\right)L(\mu_b)}{n}\right.$$
$$+\frac{n^2\psi'''_n}{6}+\frac{n\psi''_n(1+4\gamma_E n)}{2}+\psi'_n(n^2\psi'_n+2n(1+3\gamma_E)-5)-$$
$$\frac{\psi_n(n\psi_n+3(n-1)+4\gamma_E n)}{n}+\frac{(6-5n+n^2+2n^3\zeta_3-n^4\zeta_4)}{n^2}+$$
$$\left.\frac{2\gamma_E(2n^3\zeta_3-n^2\zeta_2-\frac{3}{2}+n)}{n}+4n^2S_3(n)-2nS_2(n)\right]+$$
$$(C_F\alpha_s)^2\left[-\frac{37}{24n^2}-\left(\frac{2}{3}+\frac{C_A}{C_F}\right)\left(\ln\left(\frac{C_F\alpha_s m}{2n\mu_{\rm fact}}\right)+\psi_n+\gamma_E-\frac{1}{n}\right)\right]\Bigg\}. \tag{69}$$

In the above expression, $\mathcal{K}(\mu_{\rm hard},\mu_{\rm fact})$ stands for the NNLO hard renormalization factor given explicitly in Eq.(62).

VII. THEORETICAL MOMENTS AND NUMERICAL ANALYSIS OF SUM RULES

The theoretical moments can be conveniently separated into the contributions of the perturbative resonances and of the perturbative continuum:

$$\mathcal{M}_n = \mathcal{P}_n + \mathcal{C}_n. \tag{70}$$

The resonance contribution reads:

$$\mathcal{P}_n = 6N_c\pi^2 \left(\frac{M_1}{2m}\right)^{2n} \sum_{k=1}^{\infty} \frac{|\Psi_k|^2}{m^3\left(1+\frac{E_k}{2m}\right)^{2n+1}}, \tag{71}$$

and the continuum contribution is defined as the integral of the function $R(s)/s^{n+1}$ over s (see Eq.(58)) taken above the threshold.

We stress that the above expression for the moments differs from the result one gets, merely integrating the corrections to the Green function. The difference is due to the fact, that in Eq.(71), we calculate the corrections separately to the numerator and the denominator. Working in the limit $\sqrt{n}\alpha_s \sim 1$, it is possible to expand the denominators in Eq. (71) around their values for the exact Coulomb problem; this would produce (parametrically) an $\mathcal{O}(\alpha_s)$ corrections to the moments. However, there is a serious numerical difference between the expanded and not expanded denominators. The origin of the problem is related to the large values of β_0 and $a_{1,2}$ entering the potential. This effectively translates into the large values of the corrections to the energy levels; for this reason, the expansion of the denominators is not justified in our opinion.

In contrast to the contribution of the perturbative resonances to the moments of the spectral function, the contribution of the continuous spectrum to the moments behaves nicely, as far as its perturbative expansion is concerned. The contribution of the perturbative continuum to the theoretical moments is obtained by numerical integration.

For numerical analysis of the sum rules, we use the value of the strong coupling constant $\alpha_s(M_Z)$ equal to the world average value $\alpha_s(M_Z) = 0.118$. This value of the strong coupling constant is evolved down to a required scale μ using the two–loop renormalization group evolution equation. We will later comment on the sensitivity of our results to the value of the strong coupling constant at the Z–resonance.

We also parameterize the unknown contribution of the experimental continuum $R_c(s)$ in Eq.(3) by a constant, which we vary between 0 and 2. The value of s_0 in Eq.(3) equals to $(2 \times 5.927 \text{ GeV})^2$, i.e. the continuum contribution starts at the threshold of the open $B\bar{B}$ production. To suppress the influence of this unknown contribution we have to go to rather high values of n. We have chosen n equal to $14, 16, 18$, for our analysis.

We fix the values of the hard and factorization scales at 5 GeV and examine the value of the b-quark mass as a function of the soft scale $\mu_{\rm soft}$. Our results are presented in Table 1. The values of the kinetic mass at $\mu_Q = 1$ GeV are found using Eq.(7) treated with the necessary accuracy.

The last column in Table 1 demonstrates how the perturbation theory works for the theoretical moment $\mathcal{M}_{14}$ at LO, NLO and NNLO if the NNLO value of the kinetic mass is

Scales	Order of PT	14		16		18		PT for $\mathcal{M}_{14}$
		$m_{\rm pole}$	$m_{\rm kin}$	$m_{\rm pole}$	$m_{\rm kin}$	$m_{\rm pole}$	$m_{\rm kin}$	for NNLO $m_{\rm kin}$
$\mu_{\rm soft} = 4.5$ GeV	LO	4.69	4.57	4.7	4.57	4.7	4.575	0.97
$\mu_{\rm hard} = 5$ GeV	NLO	4.74	4.49	4.75	4.50	4.76	4.51	0.61
$\mu_{\rm fact} = 5$ GeV	NNLO	4.89	4.51	4.90	4.52	4.91	4.53	0.69
$\mu_{\rm soft} = 3.5$ GeV	LO	4.73	4.59	4.73	4.59	4.73	4.595	0.95
$\mu_{\rm hard} = 5$ GeV	NLO	4.77	4.50	4.78	4.511	4.79	4.52	0.55
$\mu_{\rm fact} = 5$ GeV	NNLO	4.95	4.54	4.96	4.55	4.96	4.55	0.69
$\mu_{\rm soft} = 2.5$ GeV	LO	4.79	4.63	4.79	4.63	4.79	4.63	0.87
$\mu_{\rm hard} = 5$ GeV	NLO	4.82	4.505	4.83	4.517	4.84	4.525	0.40
$\mu_{\rm fact} = 5$ GeV	NNLO	5.08	4.595	5.08	4.595	5.09	4.6	0.69
$\mu_{\rm soft} = 2$ GeV	LO	4.84	4.67	4.84	4.666	4.84	4.66	0.72
$\mu_{\rm hard} = 5$ GeV	NLO	4.84	4.49	4.85	4.505	4.86	4.514	0.24
$\mu_{\rm fact} = 5$ GeV	NNLO	5.21	4.66	5.21	4.66	5.21	4.66	0.69

TABLE I. The kinetic mass $m_{\rm kin}$ for $\mu_Q = 1$ GeV as a function of the soft renormalization scale for the moments $n = 14, 16, 18$ and successive approximations for $\mathcal{M}_{14}$ evaluated for NNLO $m_{\rm kin}$.

used as an input. For comparison we quote here also the values of the $\mathcal{M}_{14}$ moment for the pole mass, which corresponds to the formal limit $\mu_Q \to 0$ in our approach. For $\mu_{\rm soft} = 3.5$ GeV the NNLO pole mass equals to 4.95 GeV. Calculating $\mathcal{M}_{14}$ with this mass we obtain: $\mathcal{M}_{14}^{\rm LO} = 0.2$, $\mathcal{M}_{14}^{\rm NLO} = 0.25$ and $\mathcal{M}_{14}^{\rm NNLO} = 0.69$.

From Table 1 one can see two things – the perturbation theory for the pole mass behaves in a way, that does not show any sign of convergence; the NNLO corrections normally exceed the NLO ones. Moreover, the pole mass strongly depends on the soft renormalization scale. This picture is consistent with the expectation of the irreducible ambiguity of order $\Lambda_{\rm QCD}$ in the pole mass.

For the low-scale mass the situation is different in both respects. The first terms of the perturbation series are sign alternating (if taken seriously, this feature signals that we are on the right way). Also, the low-scale running mass exhibits only a moderate dependence on $\mu_{\rm soft}$ in a relatively wide range of the soft renormalization scale. The width of this range depends on the order of perturbation theory we consider; it also depends on the initial value of $\alpha_s(M_z)$. The most stable picture emerges at the NLO, while the inclusion of the NNLO effects makes the result less stable. This partial loss of stability is the consequence of the very large value of the second order correction a_2 to the perturbative quark antiquark potential.

If the sign alternating behavior of the perturbation series for $m_{\rm kin}$ is taken seriously, one can try to perform some transformation of the perturbation series to accelerate the convergence. One of numerous options is the Euler transformation. It is interesting to observe that this transformation indeed brings the values of $m_{\rm kin}$ obtained for various values of $\mu_{\rm soft}$ closer to each other.

The Euler transformation works in the following way. Imagine we have a series $f(z) = \sum (-1)^n c_n z^n$. Then the faster convergent approximation for $f(z)$ is given by:

$$f(z) = \frac{1}{1+z}\left(c_0 - (c_1 - c_0)\left(\frac{z}{1+z}\right) + (c_2 - 2c_1 + c_0)\left(\frac{z}{1+z}\right)^2 + ...\right). \qquad (72)$$

We restricted our consideration to two orders of perturbation theory which we can use to determine the expression for the mass.

We then identify z in the previous formula with $\alpha(\mu_{\rm soft})$. Then we use the results in Table 1 for $n = 16$ and $\mu_{\rm soft} = 4.5,\ 2.5,\ 2$ GeV. For the sake of illustration, we present such calculation for $\mu_{\rm soft} = 4.5$ GeV:

$$\tilde{m} = 4.57 - 0.07 + 0.02 = 4.57\left(1 - 0.07\alpha_s + 0.09\alpha_s^2\right), \qquad \alpha_s = \alpha_s(4.5) = 0.22. \qquad (73)$$

We then use Eq.(72) and the above formula to obtain a faster convergent series:

$$m_{\rm kin} = \frac{4.57}{1+\alpha_s}\left(1 + 0.93\frac{\alpha_s}{1+\alpha_s} + 0.95\frac{\alpha_s^2}{(1+\alpha_s)^2} + ...\right) = 4.49 \text{ GeV}. \qquad (74)$$

The result does not change notably, as compared to the "naive" summation of the α_s series, indicating that in this case the numerical value of α_s is fairly small.

In the same way, we obtain the new values of the kinetic masses for the $\mu_{\rm soft} = 2.5$ and 2 GeV. The results are: for $\mu_{\rm soft} = 2.5$ GeV, we obtain $m_{\rm kin} = 4.52$ GeV and for $\mu_{\rm soft} = 2$ GeV, $m_{\rm kin} = 4.53$ GeV.

Clearly, such transformation cannot be rigorously justified; however, the fact that the numbers come closer to each other looks gratifying. Moreover, both numbers appear to become closer to the value of the NNLO mass, which can be obtained by examining the region of relative stability $\mu_{\rm soft} > 2.5 - 3$ GeV, which we use below to estimate the value of the b quark mass.

Let us also comment on how the choice of the value of $\alpha_s(M_Z)$ is reflected on our result. The important point is that this dependence is rather moderate, since the change in the initial value of $\alpha_s(M_Z)$ is roughly equivalent to the change in $\mu_{\rm soft}$. As we always work in the region where the dependence of $m_{\rm kin}$ on the normalization scale of the coupling constant is relatively weak, the same equally applies to the dependence on the initial value of α_s at the Z–resonance. The dependence on the factorization scale is much weaker than on the soft renormalization scale and amounts to a variation of at most 20 MeV in value of the kinetic mass.

We arrive finally at the following estimate for the kinetic mass extracted from the QCD sum rules:

$$m_{\rm kin}(1\text{GeV}) = 4.56 \pm 0.06 \text{ GeV}. \qquad (75)$$

We stress, that the error in the above estimate is primarily of the theoretical origin. The experimental errors in the masses and electronic decay widths of the Υ resonances, as well as a poor knowledge of the continuum part of the observable spectrum, are minor effects as compared with, e.g., the soft scale dependence of the kinetic mass. For the above estimate, we use our results for $\mu_{\rm soft}$ between 4.5 and 2.5 GeV. For lower scales, the perturbation series for the moments do not look reliable enough.

After the value of the pole mass is found, one can obtain the estimate of the $\overline{MS}$ mass $\bar{m}$. To order $\mathcal{O}(\alpha_s^2)$ the corresponding equation was given in [16]. One obtains:

$$\bar{m}(\bar{m}) = 4.20 \pm 0.1 \text{ GeV}. \tag{76}$$

Using Eq. (7), one can derive the evolution equation with respect to μ_Q and calculate the kinetic mass at different normalization scales. The only thing to be remembered is that a choice of the normalization scale μ_Q is limited by two inequalities: $\Lambda_{\rm QCD} \ll \mu_Q \ll m$. From this point of view, the pole mass, which formally corresponds to the limit $\mu_Q \to 0$, is seen to be a completely artificial notion, since it includes a nonperturbative contribution treated in terms of the perturbation theory.

Our NNLO results may look incomplete since we use relation (7) between the pole and kinetic masses, which is valid to $\mu_Q\alpha_s^2$ order, while formally one needs to know this relation more accurately, to $\mu_Q\alpha_s^3$ order. However, a careful examination based on the BLM–estimate (8) of the $\mathcal{O}(\mu_Q\alpha_s^3)$ terms, shows that unknown corrections in that order in the relation between the pole mass and the kinetic mass cannot drastically change our results for the kinetic mass in the NNLO approximation.

In any case, working with the values of the $\mu_{\rm soft}$ where perturbation theory seems to be reliable, we think we can provide a reasonable estimate for the value of the low-scale running mass to NNLO.

VIII. CONCLUSIONS

In this paper, we have determined the b quark low-scale running mass [12] from the analysis of the QCD sum rules in the next-to-next-to-leading order. We have shown that the use of this mass significantly improves the convergence of the perturbation series for the moments of the spectral density. As the result of our analysis we obtain the value of the kinetic mass normalized at 1 GeV: $m_{\rm kin}(1\text{GeV}) = 4.56 \pm 0.06$ GeV and the corresponding value of the $\overline{MS}$ mass $\bar{m}$: $\bar{m}(\bar{m}) = 4.20 \pm 0.1$ GeV.

In our opinion, the pole mass of the b quark cannot be reliably determined from the sum rule analysis. We have shown, that the NNLO order corrections to the pole mass are typically larger than the NLO ones. Also the value of the pole mass of the b quark is very sensitive to the scale of the strong coupling constant, that is used in the analysis. We think that these features are in accord with the fact that the pole mass of the quark cannot be reliably defined theoretically and suffers from an irreducible ambiguity of the order of $\Lambda_{\rm QCD}$ [9,10].

As a byproduct of our study we have obtained the NNLO analytical expression for the cross section $e^+e^- \to Q\bar{Q}$ of the quark antiquark pair production in the threshold region. We have also given the NNLO expressions for the energy levels and the wave functions at the origin for the ${}^1S_3$ bound states of $Q\bar{Q}$.

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