Bottom Quark Mass from $\Upsilon$ Mesons:
Charm Mass Effects

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Abstract
The effects of the finite charm quark mass on bottom quark mass determinations from $\Upsilon$ sum rules are examined in detail. The charm quark mass effects are calculated at next-to-next-to-leading order in the non-relativistic power counting for the $\Upsilon$ sum rules and at order $\alpha_s^3$ for the determination of the bottom $\overline{\text{MS}}$ mass. For the bottom 1S mass, which is extracted from the $\Upsilon$ sum rules directly, we obtain $M_{b^{1S}} = 4.69 \pm 0.03$ GeV with negligible correlation to the value of the strong coupling. For the bottom $\overline{\text{MS}}$ mass we obtain $M_{b^{1S}}(\overline{\text{MS}}) = 4.17 \pm 0.05$ GeV taking $\alpha^{(n_f=5)}_s(M_Z) = 0.118 \pm 0.003$ as an input. Compared with an analysis where all quarks lighter than the bottom are treated as massless, we find that the finite charm mass shifts the bottom 1S mass, $M_{b^{1S}}$, by about $-20$ MeV and the $\overline{\text{MS}}$ mass, $M_{b}(\overline{\text{MS}})$, by $-30$ to $-35$ MeV.

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1 Introduction

Precise and accurate determinations of the bottom quark mass parameter are mainly motivated by current and future B physics experiments, which aim at improved measurements of the Cabibbo–Kobayashi–Maskawa (CKM) matrix elements. This will hopefully get us closer to an understanding of the origin of flavour mixing, mass generation and CP violation. A precise and accurate knowledge of the bottom quark mass (in the scheme that is appropriate for the particular application) will eliminate one source of uncertainties. In particular, for the determination of $V_{ub}$, and also $V_{cb}$, from the semileptonic B decays the bottom quark mass is important in view of the strong dependence of the total rate and certain distributions on the bottom mass parameter. Another field where a precise bottom quark mass is desirable is represented by grand unification models. Here, precise values of the $\overline{\text{MS}}$ running heavy quark masses that are determined at low energies and that are as much as possible free of uncertainties from the strong interaction at low scales can constrain the allowed parameter space for a given scenario of flavour generation.

The bottom quark mass parameter can be obtained from properties of hadrons containing one or more bottom quarks using perturbative quantum chromodynamics (QCD) or lattice methods. Recently, lattice calculations have been applied to bottom quark mass determinations from B and $\Upsilon$ meson spectra [1, 2], whereas perturbative methods using non-relativistic effective theories were applied to bottom quark mass determinations from the mass of the $\Upsilon(1S)$ [3] and sum rules for the $\Upsilon$ masses and electronic widths [4, 5, 6, 7, 8, 9, 10]. Extractions of the bottom quark $\overline{\text{MS}}$ mass at the scale $M_Z$ have also been carried out from analyses of LEP data on bottom–antibottom–gluon three-jet events [11]. The results of the bottom $\overline{\text{MS}}$ mass from these analyses have rather large uncertainties, but they have established the evolution of the $\overline{\text{MS}}$ bottom quark mass at higher scales.

Using perturbative methods, non-relativistic sum rules for the masses and electronic decay widths of $\Upsilon$ mesons, bottom–antibottom quark bound states that have photonic quantum numbers and that can be produced in $e^+e^-$ annihilations, are in principle the most reliable tool to determine the bottom quark mass. Using causality and global duality arguments, one can relate energy integrals (or “moments”) over the total cross section for the production of final states containing a bottom–antibottom quark pair in $e^+e^-$ collisions to derivatives of the vacuum polarization function of bottom quark currents at zero-momentum transfer. For a particular range of numbers of derivatives the moments are saturated by the very precise experimental data on the $\Upsilon$ mesons and, at the same time, can be calculated reliably using perturbative QCD in the non-relativistic expansion. In contrast to the bottom quark mass determination from the $\Upsilon(1S)$ mass, the sum rule analysis is practically free from model assumptions on non-perturbative effects as long as the number of derivatives that is employed is not too high. Because the moments have, for dimensional reasons, a strong dependence on the bottom quark mass, these sum rules can be used to determine the bottom quark mass to high precision.

In the most recent sum rule analyses at NNLO in the non-relativistic expansion [8, 9, 10] special care was taken to consistently eliminate the strong linear sensitivity to small momenta and the associated (artificially) large perturbative corrections that were contained in previous analyses that employed the bottom quark pole mass. This was achieved by implementing bottom quark short-distance mass definitions into the moments that were constructed, particularly for the situation where the bottom quark is very close to its mass shell. For the implementation of these masses the systematic cancellation of the linear infrared-sensitive contributions and the compliance with the non-relativistic power counting had to be ensured in each order of perturbation theory. Melnikov–Yelkhovsky [8] used
the kinetic mass, Hoang [9] the 1S mass and Beneke–Signer [10] the PS mass. These “low-virtuality short-distance masses” can be used directly for other processes where the bottom quark virtuality is small with respect to its mass. In semileptonic B meson partial rates, for example, they lead to a very well behaved perturbative expansion (see e.g. Ref. [9, 12]). For situations where the bottom quark is very off-shell, on the other hand, the $\overline{\text{MS}}$ mass definition is the appropriate one. Starting from the low-virtuality short-distance bottom masses the previously mentioned analyses obtained $M_b(M_b) = 4.2 \pm 0.1$ GeV [8], $4.20 \pm 0.06$ GeV [9] and $4.25 \pm 0.08$ GeV [10] for the bottom $\overline{\text{MS}}$ mass. These results represent determinations of the bottom $\overline{\text{MS}}$ mass at order $\alpha_s^3$ in the usual loop expansion of perturbative QCD. The results are compatible with each other and also with the most recent lattice calculations (see Ref. [2] for a convenient compilation of results obtained after 1994). The uncertainties are considerably smaller than $\Lambda_{\text{QCD}}$ and amount to about 2%. It will be the aim of future analyses to further reduce the uncertainty, to maybe 1% or less, i.e. to an amount of a few times 10 MeV. Thus, it is mandatory to account for effects that can lead to for shifts of several times 10 MeV.

One effect, which has been entirely neglected in all previous sum rule analyses, is coming from the masses of those quarks that are lighter than the bottom, most importantly the charm quark. The massless approximation for the light quarks is a good one, provided that the light quark mass is much smaller than any of the relevant dynamical scales. In this case it is legitimate to simply expand in the light quark mass. Because all linear sensitivity to small momenta is eliminated by the use of a short-distance bottom quark mass, the first non-vanishing correction to the massless limit is of order $(\alpha_s/\pi)^2 m^2_{\text{light}}/M_b$, where $m_{\text{light}}$ is the light quark mass. Even for the charm quark this would amount to a shift of only a few MeV in the bottom quark mass and could be safely neglected. However, in order to judge whether the massless approximation is really justified, one needs to compare the light quark masses with the scales that are relevant to the non-relativistic bottom–antibottom quark dynamics that is encoded in the moments. There are two issues that make the effects of light quark masses, and of the charm quark mass in particular, a subtle problem: one is specific to the extraction of the bottom quark $\overline{\text{MS}}$ mass from the non-relativistic sum rules and the other exists for any process that is calculated at large orders of perturbation theory.

The issue that is specific to the dynamics of the non-relativistic bottom–antibottom pair encoded in the moments arises from the fact that the inverse Bohr radius, $M_b\alpha_s$, is a relevant dynamical scale. Because the inverse Bohr radius is about the same as the mass of the charm quark, it is a priori not allowed to expand in the charm quark mass. Rather, the effects of the charm quark mass have to be treated exactly, leading to a non-trivial dependence on the ratio of the charm quark mass and the inverse Bohr radius. In Ref. [13] it has been shown that this leads to an incomplete cancellation of linear charm quark mass terms $\propto \alpha_s^2 m_{\text{charm}}$ in the relation between the bottom $\overline{\text{MS}}$ and 1S masses. The resulting shift in the $\overline{\text{MS}}$ mass $M_b(M_b)$ was estimated to be around $-20$ MeV, based on a NLO calculation (which corresponds to an order $\alpha_s^2$ accuracy in the $\overline{\text{MS}}$ mass). If an expansion in the charm quark mass would be allowed, all linear charm quark mass terms would cancel exactly. The large size of the shift caused by the incomplete cancellation of the linear charm quark mass term comes from the fact that the linear charm quark mass term is enhanced. Technically, this happens because linear light quark mass terms represent non-analytic terms (in the square of the mass) that are multiplied by a factor $\pi^2$, and because the scale of the strong coupling governing them is the light quark mass and not the bottom mass. Physically, this happens because light quark masses act as an infrared cutoff for the gluon line in which the light quark loops are inserted. A linear sensitivity to small momenta is, after expansion, reflected by a non-analytic, linear dependence on the light quark mass. Because this
linear, non-analytic dependence can only arise from momenta of the order of the light quark mass, the strong coupling multiplying the linear terms is renormalized at the light quark mass. Thus, the masses of the light quarks work in complete analogy to the infinitesimally small fictitious gluon mass that is sometimes used in standard renormalon analyses. The difference is that the light quark masses are not fictitious, but finite numbers that are given by experimental data. Whether we are allowed to expand in them (or not) depends on their relation to the dynamical scales of the problem.

The other, more general issue is associated with the fact that QCD perturbation theory at large orders of perturbation theory becomes dominated by exponentially decreasing momenta. This is the origin of the divergent asymptotic behaviour of QCD perturbation theory associated to the so-called “infrared renormalons” [14, 15, 16]. This means that the genuine effects from light quarks with finite masses effectively decouple, as from a certain order, and that the large order asymptotic behaviour is considerably affected by the masses of the light quarks [17]. In fact, at large orders of perturbation theory, the difference between the massless approximation for light quarks and a calculation that includes the light quark masses becomes arbitrarily large because the evolution of the strong coupling differs in the two cases for momenta of order or below a specific light quark mass. Even at intermediate (i.e. phenomenologically relevant and calculable) orders, however, the effective decoupling of light quarks can lead to considerable deviations from the massless approximation, if the perturbative coefficients are already dominated by sufficiently small momenta. The effective decoupling is therefore not just a purely academic issue.

From the issues mentioned above we can expect the following qualitative effects coming from the finite charm quark mass in the bottom \( \overline{\text{MS}} \) mass obtained from the bottom 1S mass: the largest correction arises at order \( \alpha_s^2 \) from the fact that one can expand in the charm quark mass in the bottom pole–\( \overline{\text{MS}} \) mass relation, but not in the pole–1S mass relation [13]. The higher order charm quark mass corrections should decrease because the importance of the dynamical scales \( M_b \), and \( M_b \alpha_s \) becomes less prominent as the dominating momenta decrease exponentially. This means that the charm mass corrections are under control and can be calculated reliably\(^1\). From the light quarks other than the charm, we do not expect any sizeable corrections because, at the accessible orders of perturbation theory, their masses are simply too small to make any of the previous considerations relevant. However, a quantitative statement about the actual size and behaviour of the charm mass corrections can only be made through an actual calculation. In addition, it is mandatory to assess how the finite charm quark mass affects the extraction of the bottom 1S mass from the \( \Upsilon \) sum rules. For the bottom \( \overline{\text{MS}} \) mass the corrections might either add up or cancel at the end. In the former case the charm quark mass effects for the final value of \( \overline{\text{MS}}(\Upsilon) \) might be larger than the 20 MeV estimate that has been obtained in the NLO (or order \( \alpha_s^2 \)) analysis of Ref. [13].

In this paper we determine the charm mass corrections at order \( \alpha_s^3 \) in the bottom \( \overline{\text{MS}} – 1S \) mass relation as well as for the bottom 1S mass determination from the \( \Upsilon \) meson sum rules at NNLO in the non-relativistic expansion. This includes the calculation of the NNLO light quark mass corrections to the perturbative contributions of the \( \Upsilon(1S) \) mass in terms of the pole mass, and the order \( \alpha_s^3 \) light quark mass corrections in the heavy quark pole–\( \overline{\text{MS}} \) mass relation. The latter corrections are determined in the linear light quark mass approximation because an expansion in the light quark masses is allowed in that case. The determination of the linear order \( \alpha_s^3 \) light quark mass corrections

\(^1\)We emphasize that this statement is not correct if one attempts a determination of the bottom quark pole mass. Its well-known ambiguity of order \( \Lambda_{\text{QCD}} \) is directly reflected in an uncontrollable behaviour of the charm mass corrections. This is demonstrated in Sec. 5.2.
is based on the conjecture that linear light quark mass terms are absent in the total static energy of a heavy quark-antiquark pair. As far as the bottom $\overline{\text{MS}}$–1S mass relation is concerned, we also attempt to estimate the order $\alpha_s^4$ charm mass corrections based on a calculation of the NNNLO (N$^3$LO) perturbative corrections in the $\Upsilon$(1S) mass, in the large-$\beta_0$ approximation. For the $\Upsilon$ sum rules we determine charm mass corrections at NLO and NNLO in the non-relativistic expansion, where we neglect the double-insertion contributions coming from second order Rayleigh–Schrödinger time-independent perturbation theory at NNLO. For all results we discuss in detail the behaviour of the light quark mass corrections. It is demonstrated that the effects coming from the masses of up, down and strange quarks can, as expected, be neglected.

We note that, although the effects of the light quark masses can be presented in a straightforward way in the framework of effective theories for non-relativistic heavy quark–antiquark pairs, we will not give such a presentation in this work. This is because we feel the discussion of the many interesting aspects of light quark mass effects, which do not depend at all on the concepts of effective theories, would become cumbersome. We also emphasize that all results presented in this work are given in the convention that the evolution of the strong $\overline{\text{MS}}$ coupling includes the light quarks with finite mass, i.e. we use $\alpha_s^{(n_l=4)}$ for our results for the bottom quark masses. We do this because all previous analyses, which neglected light quark masses, naturally used this definition of $\alpha_s$. It is therefore easy to update the previous analyses by simply adding the new corrections determined in this work. In this context we also note that many conclusions and statements made in this work about the behaviour and the size of the charm mass corrections at the different orders are not adequate if $\alpha_s^{(n_l=3)}$ is chosen as the definition of the strong coupling, since this would lead to a reshuffling of corrections. The final numbers for the bottom 1S and $\overline{\text{MS}}$ masses, however, do not depend on this choice.

The plan of this paper is as follows: in Sec. 2 we briefly review the ingredients needed to describe the heavy-quark–antiquark dynamics at NNLO in the non-relativistic expansion for massless light quarks and the result for the NNLO light quark mass corrections to the static potential obtained earlier by Melles [18, 19]. The results by Melles are rewritten in a more convenient dispersion relation representation. The limit of vanishing light quark mass and the resulting linear light quark mass terms are examined, and the prediction for the order $\alpha_s^3$ linear light quark mass corrections in the heavy quark pole–$\overline{\text{MS}}$ mass relation is made. The quality of the linear light quark mass approximation in the heavy quark pole–$\overline{\text{MS}}$ mass relation is analysed in Sec. 3. In Sec. 4 the NNLO light quark mass corrections to the relation between the heavy quark 1S and pole masses are presented, and in Sec. 5 the results from Secs. 3 and 4 are combined to derive the order $\alpha_s^3$ (or NNLO) relation between the heavy quark $\overline{\text{MS}}$ and 1S masses, where light quark mass effects are taken into account. The upsilon expansion [20], a prescription for a modified perturbative expansion that allows for a consistent derivation of the $\overline{\text{MS}}$–1S mass relation in each order, is reviewed. The size of the charm mass corrections is analysed and an estimate for the order $\alpha_s^4$ (or N$^3$LO) charm mass corrections is given. In Sec. 6 we determine the NNLO light quark mass corrections to the moments of the $\Upsilon$ sum rules, and in Sec. 7 we carry out the numerical analysis to determine the bottom 1S mass from fitting theoretical and experimental moments. The relation of our result for the bottom 1S mass to the mass of the $\Upsilon$(1S) meson is discussed, and the result for the bottom $\overline{\text{MS}}$ mass is presented. All results are discussed focusing on the charm mass effects. Section 8 contains a summary. Attached to the paper are five appendices: in App. A details on the calculations of the NNLO light quark mass corrections to the mass of the $J^{PC} = 1^{--}, 3S_1$ heavy perturbative quarkonium ground state are given. Appendix B contains the calculation of the N$^3$LO perturbative corrections to the mass of the
heavy quarkonium ground state in the large-$\beta_0$ approximation. In App. C the results for the order $\alpha_s^4$ (or $N^3$LO) perturbative corrections to the heavy quark $\overline{MS}$–$1S$ mass relation are derived in the large-$\beta_0$ approximation. Appendix D contains exact analytic results for the order $\alpha_s^3$ light quark mass corrections to the heavy quark pole–$\overline{MS}$ mass relation coming from vacuum polarization insertions, and App. E gives some formulae for the corrections to the moments of the $\Upsilon$ sum rules from massless light quarks.

2 Considerations on the Static Potential including Light Quark Mass Effects

The static potential represents the central quantity needed to determine the effects of the masses of light quarks on the dynamics of a perturbative non-relativistic heavy-quark–antiquark pair. In this section we discuss the corrections to the static potential up to NNLO in the non-relativistic expansion coming from the mass of a light quark.

2.1 Massless Light Quarks

At NNLO in the non-relativistic expansion, the dynamics of a perturbative heavy-quark–antiquark pair\(^2\) represents a pure 2-body problem and can be described by a textbook-like Schrödinger equation that contains the kinetic energy term and a time-independent instantaneous potential. In configuration space representation, the Schrödinger equation has the form (\(E = \sqrt{s} - 2M_Q^{\text{pole}}\)):

\[
\left(-\nabla^2 M_Q^{\text{pole}} - \frac{1}{4(M_Q^{\text{pole}})^3} \right) \left[ V_{c}^{\text{LO}}(r) + V_{c}^{\text{NLO}}(r) + V_{c}^{\text{NNLO}}(r) + V_{BF}(r) + V_{\text{NA}}(r) \right] - E \right) \times G(r, r', E) = \delta^{(3)}(r - r'),
\]

where \(M_Q^{\text{pole}}\) is the heavy quark pole mass and \(s\) the squared centre-of-mass energy. Although the use of the pole mass is a bad choice for a phenomenological analysis, because of its strong sensitivity to small momenta, we will use it for intermediate calculations because it leads to the simple form of the Schrödinger equation shown in Eq. (1). The terms \(V_{c}^{\text{LO}}, V_{c}^{\text{NLO}}\) and \(V_{c}^{\text{NNLO}}\) represent the static (Coulomb) potential at LO (order \(v^2 \sim \alpha_s^2\)), NLO (order \(v^3 \sim \alpha_s^3\)) and NNLO (order \(v^4 \sim \alpha_s^4\)), respectively, in the non-relativistic power counting, while \(V_{BF}\) is the Breit-Fermi potential known from positronium and \(V_{\text{NA}}\) is a non-Abelian potential coming from a non-analytic gluonic correction to the exchange of a Coulomb gluon; \(V_{BF}\) and \(V_{\text{NA}}\) are of NNLO. The kinetic energy terms \(-\nabla^2/M_Q^{\text{pole}}\) and \(-\nabla^4/4(M_Q^{\text{pole}})^3\) are of LO and NNLO, respectively. Treating all \(n_l\) quarks that are lighter than the heavy quark as massless the individual potentials read (\(a_s \equiv \alpha_s(n_l)(\mu), r \equiv |r|, \tilde{\mu} \equiv e^{\gamma_E} \mu, C_A = 3, C_F = 4/3, T = 1/2\))

\[
V_{c}^{\text{LO}}(r) = -\frac{C_F a_s}{r},
\]

\[
V_{c,\text{massless}}^{\text{NLO}}(r) = V_{c}^{\text{LO}}(r) \left(\frac{a_s}{4\pi}\right) \left[ 2\beta_0 \ln(\tilde{\mu} r) + a_1 \right],
\]

\(^2\)In this context “perturbative” means that the heavy quark mass, \(M_Q\), is large enough, such that the hierarchy \(M_Q \gg M_Q v \gg M_Q v^2 \gg \Lambda_{\text{QCD}}\) holds, \(v\) being the heavy quark velocity.
\begin{align*}
V_{c,\text{massless}}^{\text{NNLO}}(r) &= V_c^{\text{LO}}(r) \left( \frac{a_s}{4\pi} \right)^2 \left[ \beta_0^2 \left( 4 \ln^2(\mu r) + \frac{\pi^2}{3} \right) + 2 \left( 2 \beta_0 a_1 + \beta_1 \right) \ln(\mu r) + a_2 \right], \quad (4) \\
V_{BF}(r) &= \frac{C_F a_s \pi}{(M_{\text{pole}}^2)^2} \left[ 1 + \frac{8}{3} \delta_{(3)}(r) \right] + \frac{C_F a_s}{2(M_{\text{pole}}^2)^2} \frac{1}{r} \left[ \nabla^2 + \frac{1}{r^2} \text{r} \nabla \right] \\
&\quad - \frac{3 C_F a_s}{(M_{\text{pole}}^2)^2} \frac{1}{r^3} \left[ \frac{1}{3} S_b S_b - \frac{1}{r^2} \left( S_b \text{r} \right) \left( S_b \text{r} \right) \right] + \frac{3 C_F a_s}{2(M_{\text{pole}}^2)^2} \frac{1}{r^3} L \left( S_b + S_b \right), \quad (5) \\
V_{\text{NA}}(r) &= -\frac{C_A C_F a_s^2}{2M_{\text{pole}}^2} \frac{1}{r^2}, \quad (6)
\end{align*}

where

\begin{align*}
\beta_0 &= \frac{11}{3} C_A - \frac{4}{3} T n_l, \\
\beta_1 &= \frac{34}{3} C_A^2 - \frac{20}{3} C_A T n_l - 4 C_F T n_l, \\
a_1 &= \frac{31}{9} C_A - \frac{20}{9} T n_l, \\
a_2 &= \left( \frac{4343}{162} + 4 \pi^2 - \frac{\pi^4}{4} + \frac{22}{3} \zeta_3 \right) C_A^2 - \left( \frac{1798}{81} + \frac{56}{3} \zeta_3 \right) C_A T n_l \\
&\quad - \left( \frac{55}{3} - 16 \zeta_3 \right) C_F T n_l + \left( \frac{20}{9} T n_l \right)^2, \quad (10)
\end{align*}

\( S_b \) and \( S_b \) are the bottom and antibottom quark spin operators, \( L \) is the angular momentum operator, and \( \gamma_E = 0.57721566... \) is the Euler–Mascheroni constant. The constants \( a_1 \) and \( a_2 \) have been calculated in Refs. [21, 22] and Refs. [23, 24], respectively. For the determination of the corrections coming from a finite light quark mass in physical heavy-quark–antiquark properties at NNLO, the expressions for \( V_c^{\text{LO}} \) and \( V_{c,\text{massless}}^{\text{NNLO}} \) will be needed explicitly. The superscript “\( n_l \)” shown by the strong coupling indicates that the results are written in terms of the strong coupling that evolves with \( n_l \) active quark flavours. If the light quark masses are much smaller than the typical inverse distances of the heavy quarks, this convention is the only sensible one, as it avoids the appearance of logarithms of the light quark masses.

### 2.2 Effects of a Light Quark Mass

From the explicit dependence of Eqs. (2)–(6) on the number of light quarks \( n_l \), one can easily see that only the static potential at NLO and NNLO acquire additional corrections from a finite light quark mass. In the following we present the corrections to the static potential at NLO and NNLO for the case that only one light quark species has a finite mass \( m \), whereas the \( n_l - 1 \) other quark species are treated as massless. For convenience we adopt the pole mass definition for the light quark mass \( m \). The generalization to other light quark mass definitions, and to the case where more than one of the \( n_l \) light quarks have a finite mass, is straightforward. We note that all final results for the light quark mass corrections presented in this work will be expressed in terms of the light quark \( \overline{\text{MS}} \) mass \( \overline{m(m)} \).
Figure 1: NLO contribution to the static potential coming from the insertion of a one-loop vacuum polarization of a light quark with finite mass.

At NLO the light quark mass corrections to the static potential arise from the insertion of the light quark self energy into the gluon line of the LO static potential (see Fig. 1). In momentum space representation the NLO static potential including the light quark mass corrections reads ($a_s = \alpha_s(\mu)$)

$$\tilde{V}^{NLO}_{c}(p) = \tilde{V}^{NLO}_{c,\text{massless}}(p) + \delta\tilde{V}^{NLO}_{c}(p),$$  

(11)

$$\tilde{V}^{NLO}_{c,\text{massless}}(p) = \tilde{V}^{LO}_{c}(p) \left( \frac{a_s}{4\pi} \right) \left[ -\beta_0 \ln \left( \frac{p^2}{\mu^2} \right) + a_1 \right],$$  

(12)

$$\delta\tilde{V}^{NLO}_{c}(p) = \tilde{V}^{LO}_{c}(p) \left( \frac{a_s}{4\pi} \right) \frac{4}{3} T P \left( \frac{m^2}{p^2} \right),$$  

(13)

$$\tilde{V}^{LO}_{c}(p) = -\frac{4\pi C_F a_s}{p^2},$$  

(14)

where

$$P\left( \frac{m^2}{p^2} \right) = \left[ \Pi\left( \frac{m^2}{p^2} \right) - \left( \ln \frac{p^2}{m^2} - \frac{5}{3} \right) \right],$$  

(15)

$$\Pi\left( \frac{m^2}{p^2} \right) = \frac{1}{3} - (1 - 2z) \left[ 2 - \sqrt{1 + 4z} \ln \left( \frac{\sqrt{1 + 4z} + 1}{\sqrt{1 + 4z} - 1} \right) \right]_{z = \frac{m^2}{p^2}},$$

(16)

$$f(x) = \frac{1}{x^2} \sqrt{x^2 - 1} \left( 1 + \frac{1}{2x^2} \right),$$  

(17)

We note that \( P \) also contains the subtraction of the light quark mass vacuum polarization in the limit $m \to 0$. Thus the light quark mass corrections $\delta\tilde{V}^{NLO}_{c}$ vanish for $m \to 0$ or $p^2 \to \infty$. This is a consequence of our choice to include the light quark with mass $m$ into the evolution of the strong
The dispersion relation representation for the light quark vacuum polarization function shown in Eq. (16) is quite useful because it allows for a quick determination of the light quark mass corrections in configuration space representation ($\tilde{m} = e^{\gamma_E} m$):

$$\delta V^{NLO}_{c,m}(r) = \int \frac{d^3p}{(2\pi)^3} \delta \tilde{V}^{NLO}_{c,m}(p) \exp(i p r)$$

where

$$V^{LO}_{c}(r) = \left( \frac{a_s}{3\pi} \right) \left\{ \int_1^\infty dx f(x) e^{-2mrx} + \left( \ln(\tilde{m}r) + \frac{5}{6} \right) \right\}.$$  \hspace{0.5cm} (18)

The expression in the second line of Eq. (18) (without the subtraction of the contributions for $m \to 0$) has been derived a long time ago by Serber and Ueling [25] for the effects of the electron on the QED static potential of a charged particle. The use of the dispersion relation representation for the light quark mass corrections to the static potential is advantageous for the determination of higher order terms in Rayleigh–Schrödinger perturbation theory due to the universality and simplicity of the dependence on $r$ (or $p$). The remaining dispersion integration can be carried out numerically (or if possible analytically) at the very end. We believe that this method is actually the only feasible one to determine the light quark mass corrections, particularly for the light quark mass corrections in the NNLO static potential and for multiple insertions of the NLO static potential at higher order in Rayleigh–Schrödinger perturbation theory. For the determination of the dispersion relation representation, it is a useful fact that the corrections of the light quark mass with the (pole) mass $m$ decouple (i.e. vanish for $p^2 \to 0$) if we exclude it from the evolution of the strong coupling. Up to two loops the matching relation of the strong coupling in the two schemes, where the light quark with mass $m$ is included and excluded in the evolution, reads [26]

$$\alpha^{(n_l)}_{s}(\mu) = \alpha^{(n_l-1)}_{s}(\mu) \left\{ 1 + \left( \frac{\alpha^{(n_l-1)}_{s}(\mu)}{\pi} \right) \left[ \frac{1}{6} \ln \left( \frac{\mu^2}{m^2} \right) \right] \right. \left. + \left( \frac{\alpha^{(n_l-1)}_{s}(\mu)}{\pi} \right)^2 \left[ \frac{7}{24} + \frac{19}{24} \ln \left( \frac{\mu^2}{m^2} \right) + \frac{1}{36} \ln^2 \left( \frac{\mu^2}{m^2} \right) \right] \right\}.$$  \hspace{0.5cm} (19)

Thus, after rewriting the static potential in terms of $\alpha^{(n_l-1)}_{s}$, only the subtracted dispersion integral expression remains for the corrections coming from the finite light quark mass $m$. We have used this useful fact to determine the dispersion relation representation for the light quark mass corrections to the static potential at NNLO.

At NNLO the light quark mass corrections to the static potential arise from dressing the one-loop Feynman diagram displayed in Fig. 1 with additional gluon, ghost and light quark lines, where the heavy quark lines in the resulting loops and the couplings of the heavy quarks to gluons correspond to those of static quarks [21] as they are used in Heavy-Quark Effective Theory. The corresponding diagrams were calculated numerically by Melles [18]. Fitted approximation formulae for the NNLO static potential with the corrections of a light quark mass in momentum as well as configuration space representation were given in Ref. [19]. There, the results were presented for $n_l = 1$ and using $\alpha^{(n_l=1)}_{s}$ as the definitions for the strong coupling. However, these results are somewhat cumbersome to use for bound state calculations at higher order in Rayleigh–Schrödinger perturbation theory. Using the decoupling properties of the massive light quark corrections as explained above, it is straightforward to derive the following dispersion relation representation of the light quark mass corrections to the
NNLO static potential in momentum space representation\(^3\) \((a_s = \alpha_s^{(n)}(\mu))\):

\[
\tilde{V}_c^{\text{NNLO}}(p) = \tilde{V}_c^{\text{NNLO, massless}}(p) + \delta \tilde{V}_c^{\text{NNLO}}(p), \tag{20}
\]

\[
\tilde{V}_c^{\text{NNLO, massless}}(p) = \tilde{V}_c^{\text{LO}}(p) \left( \frac{a_s}{4\pi} \right)^2 \left[ \frac{\beta_0}{2} \ln^2 \left( \frac{p^2}{\mu^2} \right) - \left( 2\beta_0 a_1 + \beta_1 \right) \ln \left( \frac{p^2}{\mu^2} \right) + a_2 \right], \tag{21}
\]

\[
\delta \tilde{V}_c^{\text{NNLO}}(p) = \tilde{V}_c^{\text{LO}}(p) \left( \frac{a_s}{4\pi} \right)^2 \left[ \frac{8}{3} T P \left( \frac{m^2}{p^2} \right) \left( -\beta_0 \ln \left( \frac{p^2}{\mu^2} \right) + a_1 \right) + \left( \frac{4}{3} T \right)^2 P^2 \left( \frac{m^2}{p^2} \right) + \frac{76}{3} T X \left( \frac{m^2}{p^2} \right) \right], \tag{22}
\]

where

\[
X \left( \frac{m^2}{p^2} \right) = \left[ \Xi \left( \frac{m^2}{p^2} \right) - \left( \ln \frac{p^2}{m^2} - \frac{161}{114} - \frac{26}{19} \zeta_3 \right) \right], \tag{23}
\]

\[
\Xi \left( \frac{m^2}{p^2} \right) = 2c_1 p^2 \int_{c_2}^{\infty} \frac{dx}{x} \frac{1}{p^2 + 4m^2 x^2} + 2d_1 p^2 \int_{d_2}^{\infty} \frac{dx}{x} \frac{1}{p^2 + 4m^2 x^2}
= c_1 \ln \left( 1 + \frac{p^2}{4c_2^2 m^2} \right) + d_1 \ln \left( 1 + \frac{p^2}{4d_2^2 m^2} \right), \tag{24}
\]

and the definition of \(P\) has been given in Eq. (15). In contrast to the approximation formulae given in Ref. [19], the contributions involving the one-loop vacuum polarization contributions coming from the light quark with mass \(m\) are exact. The remainder, which is parametrized in terms of the function \(X\), depends on the constants \(c_1, c_2, d_1\) and \(d_2\). Because \(\Xi\) vanishes for \(p^2 \to 0\) and \(X\) for \(p^2 \to \infty\), the constants satisfy the conditions \(c_1 + d_1 = 1\) and \(c_1 \ln (4c_2^2) + d_1 \ln (4d_2^2) = \frac{161}{114} + \frac{26}{19} \zeta_3\). A useful parametrization for the constants, which fulfils these conditions and keeps \(c_2\) and \(d_2\) as free parameters, is

\[
c_1 = \frac{\ln \frac{d_2}{d_2}}{\ln \frac{c_2}{c_2}}, \tag{25}
\]

\[
d_1 = \frac{\ln \frac{c_2}{c_2}}{\ln \frac{d_2}{d_2}}, \tag{26}
\]

\[
A = \exp \left( \frac{161}{228} + \frac{13}{19} \zeta_3 - \ln 2 \right). \tag{27}
\]

For the constants \(c_2\) and \(d_2\) we obtain

\[
c_2 = 0.470 \pm 0.005, \tag{28}
\]

\[
d_2 = 1.120 \pm 0.010 \tag{29}
\]

\(^3\)I thank M. Melles for checking Eqs. (22) and (30).
from fitting to the results in Eq. (30) of Ref. [19]. We assume a 1% uncertainty for $c_2$ and $d_2$, but we note that this estimate is not based on a statistical analysis. The uncertainties have been fixed by hand in an ad hoc manner taking into account the uncertainties quoted in Ref. [19] and the fact that the numerical result shown in Eq. (30) of Ref. [19] does not decouple exactly. We note that the uncertainties in the charm mass effects for the bottom mass extractions caused by the errors in $c_2$ and $d_2$ are an order of magnitude smaller than those caused by the other approximations made in this work. We therefore ignore the errors in $c_2$ and $d_2$ for the rest of this paper. Finally, the NNLO light quark mass corrections to the static potential in configuration space representation read ($a_s = a_s^{(n)}(\mu)$)

$$
\delta V_{c,m}^{\text{NNLO}}(r) = V_c^{\text{LO}}(r) \left( \frac{a_s}{3\pi} \right)^2 \left\{ \right.
- \frac{3}{2} \int_1^\infty dx f(x) e^{-2mx} \left( \beta_0 \left( \ln \frac{4m^2 x^2}{\mu^2} - \text{Ei}(2mx) - \text{Ei}(-2mx) \right) - a_1 \right) \\
+ 3 \left( \ln(\bar{m}r) + \frac{5}{6} \right) \left( \beta_0 \ln(\bar{\mu}r) + \frac{a_1}{2} \right) + \beta_0 \frac{\pi^2}{4} \right.
- \left. \int_1^\infty dx f(x) e^{-2mr} \left( \frac{5}{3} + \frac{1}{2x} \left( 1 + \frac{1}{2} \sqrt{x^2 - 1} \right) \ln \left( \frac{x - \sqrt{x^2 - 1}}{x + \sqrt{x^2 - 1}} \right) \right) \right. \\
+ \left. \int_1^\infty dx f(x) e^{-2mr} \left( \ln(4x^2) - \text{Ei}(2mr) - \text{Ei}(-2mr) - \frac{5}{3} \right) \right. \\
+ \left( \ln(\bar{m}r) + \frac{5}{6} \right)^2 + \pi^2 \left. \frac{12}{12} \right. \\
+ \left. \left[ \frac{57}{4} \left( c_1 \Gamma(0, 2c_2 mr) + d_1 \Gamma(0, 2d_2 mr) + \ln(\bar{m}r) + \frac{161}{228} + \frac{13}{19} \zeta_3 \right) \right] \right\}, \tag{30}
$$

where $\text{Ei}$ is the exponential-integral function and $\Gamma$ the incomplete gamma function, where $\Gamma(0, ca) = \int_c^\infty e^{-ax}/x \, dx$. For the exponential-integral function the relation $\text{Ei}(z) + \text{Ei}(-z) = P \int_0^{\infty} 2t e^{(1+t^2)z}/(1-t^2) \, dt$, where $P$ refers to the principal value prescription, is quite useful. We note that of the three terms in the brackets on the RHS of Eq. (30), each one vanishes individually for $m \to 0$. The first two terms incorporate all the light quark mass corrections that can be obtained from insertions of one-loop light quark vacuum polarizations.

### 2.3 Small-Distance Limit and Linear Light Quark Mass Terms

It is instructive to consider the light quark mass corrections to the static potential for the case where the distance between the heavy quark is much smaller than $1/m$, i.e. in the limit $m \ll 1/r$. In this case the light quark mass corrections to the static potential read ($a_s = a_s^{(n)}(\mu)$):

$$
\delta V_{c,m}^{\text{Lo}}(r) + \delta V_{c,m}^{\text{NNLO}}(r) \xrightarrow{m \ll 1/r} - 2C_F \left( \frac{a_s}{\pi} \right)^2 \frac{\pi^2}{8} m \left\{ 1 + 2 \left( \frac{a_s}{4\pi} \right) \left[ a_1 + \beta_0 \left( \ln \frac{\mu^2}{m^2} + 3 - 4\ln 2 \right) \right] \right. \\
+ \left. \frac{4}{45} \left( 31 - 30\ln 2 \right) + \frac{76}{3\pi} \left( c_1 c_2 + d_1 d_2 \right) \right\} + \mathcal{O}(m^2 r)
$$
\[ -2 C_F \left( \frac{a_s}{\pi} \right)^2 \frac{\pi^2}{8} m \left\{ 1 + 2 \left( \frac{a_s}{4\pi} \right) \left[ \beta_0 \left( \ln \frac{\mu^2}{m^2} - 4 \ln 2 + \frac{14}{3} \right) \right. \right. \\
\left. \left. - \frac{4}{3} \left( \frac{59}{15} + 2 \ln 2 \right) + \frac{76}{3\pi} \left( c_1 c_2 + d_1 d_2 \right) \right] \right\} \right\} + \mathcal{O}(m^2 r), \]  

(31)

where we have used the relation \( a_1 = \frac{5}{2} \beta_0 - 8 \) in the second line of Eq. (31). The order \( \alpha_s^3 \beta_0 \) term in the second line has already been derived in Ref. [13]. The leading term in the expansion, which is linear in the light quark mass\(^4\), has a number of remarkable features: it is independent of \( r \), enhanced by a factor of \( \pi^2 \), and its characteristic scale is the light quark mass \( m \) rather than the inverse of the distance \( r \). We emphasize that the linear light quark mass term cannot be obtained by first expanding Eqs. (18) and (30) in the light quark mass and carrying out the dispersion integrations (over the variable \( \xi \)) afterwards, because it contains contributions coming from large values of \( \xi \), i.e. from momenta of the order of the light quark mass or smaller (see Eq. (16)). This means that the linear mass term is of infrared origin, which explains that it represents a non-analytic expression in \( m^2 \). In fact, the linear light quark mass term is in complete analogy with the linear gluon mass term that would arise if we were give the gluon a infinitesimally small fictitious mass \( \lambda \). The linear light quark mass term at order \( \alpha_s^n \) directly corresponds to the linear gluon mass term that would be obtained at order \( \alpha_s^{n-1} \). (This can be seen from Eq. (16), using the change of variable \( \lambda^2 = 4m^2\xi^2 \).) Just as for the linear gluon mass term, the existence of the linear light quark mass term in Eq. (31) indicates that the static potential is, like the heavy quark pole mass, linearly sensitive to small momenta. Thus, the static potential also contains an \( (r\text{-independent}) \) ambiguity of order \( \Lambda_{\text{QCD}} \). This also explains why the perturbative series for the linear quark mass term is completely out of control for all light quarks, although the perturbative expansion of the static potential is most trustworthy in the small distance limit. For the charm quark the linear mass term amounts to 60 MeV at order \( \alpha_s^2 \) and to 86 MeV at order \( \alpha_s^3 \) for \( \overline{m}(m) = \mu = 1.5 \text{ GeV}, a_s = 0.36 \) and \( n_l = 4 \) indicating a very bad higher order behaviour\(^5\). (See Sec. 3 for a more detailed discussion.)

Fortunately, a linear sensitivity to small momenta and the corresponding ambiguity of order \( \Lambda_{\text{QCD}} \), is not contained in the total static energy \([30, 31, 32]\)

\[ E_{\text{stat}} = 2M_{\text{pole}} + V_c(r). \]  

(32)

In Refs. [30, 32] this was proved at one loop. The proof in Ref. [31] demonstrates this also at the two-loop level, which is sufficient for the purpose of this work. A similar proof for inclusive semileptonic B meson decays can be found in Ref. [33]. Equation (32) means that—if we are actually allowed to expand the static potential in the light quark mass—the linear light quark mass corrections are cancelled, if a short-distance mass definition is employed to describe the non-relativistic heavy-quark–antiquark dynamics. This remarkable feature allows us to determine the linear light quark mass corrections in the relation between the heavy quark pole and a short-distance mass, such as the \( \overline{\text{MS}} \)

---

\(^4\)In a non-relativistic effective field theory for heavy quarks, in which the light quark is also integrated out, the linear light quark mass term corresponds to a residual mass term operator [13]. This term accounts for the difference in the analyticity structure at low energies of the effective theory in which the light quark is integrated out and the theory in which the light quark is not integrated out. This also means that the heavy quark pole masses in both theories differ by the coefficient of the residual mass operator [27], see also the section on quark masses in Ref. [28].

\(^5\)This statement about the higher order behaviour of the linear charm quark mass terms does not depend on which convention is used for the strong coupling.
The order $\alpha_s^2$ linear light quark mass term of the static potential shown in Eq. (31) confirms the order $\alpha_s^2$ linear light quark mass term in the heavy quark pole–$\overline{\text{MS}}$ mass relation calculated earlier in Ref. [34]. The order $\alpha_s^3$ term that can be derived from Eqs. (31) and (33) has to our knowledge not been obtained before. A detailed discussion on the linear light quark mass corrections in the relation of the heavy quark pole and $\overline{\text{MS}}$ masses is given in Sec. 3.

We are now in a position to substantiate the scenario for the light quark mass corrections that we have pictured in the introduction to this work for the extraction of bottom quark masses from $\Upsilon$ mesons at intermediate orders of perturbation theory. For the light quarks up, down and strange, the badly behaved linear mass terms indeed cancel in an extraction of the bottom $\overline{\text{MS}}$ mass, because their masses are much smaller than the dynamical scales $M_b$ and $\langle 1/r \rangle \approx M_b \alpha_s$ and do not expand in them everywhere, in the same way as in the infinitesimally small gluon mass. For the charm quark, however, the expansion in its mass is allowed in the bottom quark pole–$\overline{\text{MS}}$ mass relation (because it is only governed by the scale $M_Q$), but not in quantities involving the bottom–antibottom non-relativistic dynamics described through the Schrödinger equation (1). This means that, for an extraction of the bottom $\overline{\text{MS}}$ mass from $\Upsilon$ mesons, at least some part of the large linear charm mass corrections remains uncancelled. Regarding the very bad perturbative convergence for the linear charm mass terms in Eq. (33), it is now natural to ask the question of how the remaining linear charm mass corrections will behave at higher orders. If they were to behave similarly to the linear charm mass corrections in Eq. (31), then the precision of the bottom $\overline{\text{MS}}$ mass would be forever limited to several tens of MeV. Fortunately, this is not the case because the contributions from low momenta increase at higher orders of perturbation theory. This means that the small momentum region, where the linear mass terms originate, dominates over the larger momenta. Thus, although it is formally impossible to expand in the charm mass divided by the inverse Bohr radius, the coefficients of higher powers of this ratio will decrease at higher orders, making the linear term the dominant one. In Sec. 5.2 we will demonstrate this interesting feature explicitly. For the extraction of the bottom $\overline{\text{MS}}$ mass this means that the charm mass corrections are well under control and calculable.

### 3 Light Quark Mass Corrections in the Heavy Quark Pole–$\overline{\text{MS}}$ Mass Relation

The perturbative relation between the pole and the $\overline{\text{MS}}$ mass definition of a heavy quark is a main ingredient in the determination of the bottom $\overline{\text{MS}}$ mass from data on the $\Upsilon$ mesons. The mass of a light quark leads to corrections in this relation starting at order $\alpha_s^2$, originating from the insertion of a light quark vacuum polarization into the one-loop gluon line. For a proper determination of the bottom $\overline{\text{MS}}$ mass using calculations for the non-relativistic bottom–antibottom quark dynamics at NNLO (see Eq. (1)), we need the bottom pole–$\overline{\text{MS}}$ mass relation at order $\alpha_s^3$. Here, “proper” means that the artificially large perturbative contributions coming from a linear sensitivity to small momenta...
are eliminated consistently in each order\(^6\). For massless light quarks the heavy quark pole–\(\overline{\text{MS}}\) mass relation is known analytically at order \(\alpha_s^3\). The order \(\alpha_s^2\) corrections have been determined in Ref. [34] and the order \(\alpha_s^3\) corrections in Ref. [12]. A numerical determination of the order \(\alpha_s^3\) corrections can be found in Ref. [35]. In Ref. [34] the order \(\alpha_s^2\) corrections coming from the mass of a light quark have been determined analytically for all values of the light quark mass. The light quark mass corrections at order \(\alpha_s^3\) are only known in the linear mass approximation and have been determined in Sec. 2.3 of this work. At order \(\alpha_s^3\) the relation between the pole and the \(\overline{\text{MS}}\) mass of a heavy quark for \(n_l\) light quarks, of which one has a finite pole mass \(m\), reads \((\bar{a}_s = \alpha_s^{(n_l)}(\overline{\text{M}}_Q)):\)

\[
\begin{align*}
M_Q^{\text{pole}} &= \overline{\text{M}}_Q(\overline{\text{M}}_Q) \left\{ 1 + \epsilon \left[ \delta^{(1)}(\bar{a}_s) \right] + \epsilon^2 \left[ \delta^{(2)}_{\text{massless}}(\bar{a}_s) + \delta^{(2)}_{\text{massive}}(m, \overline{\text{M}}_Q(\overline{\text{M}}_Q), \bar{a}_s) \right] \\
&+ \epsilon^3 \left[ \delta^{(3)}_{\text{massless}}(\bar{a}_s) + \delta^{(3)}_{\text{massive}}(m, \overline{\text{M}}_Q(\overline{\text{M}}_Q), \bar{a}_s) \right] + \ldots \right\}, \tag{34}
\end{align*}
\]

where the corrections for massless light quarks read

\[
\begin{align*}
\delta^{(1)} &= \frac{4}{3} \left( \frac{\bar{a}_s}{\pi} \right), \tag{35} \\
\delta^{(2)}_{\text{massless}} &= \left( \frac{\bar{a}_s}{\pi} \right)^2 \left( 13.443 - 1.0414 n_l \right), \tag{36} \\
\delta^{(3)}_{\text{massless}} &= \left( \frac{\bar{a}_s}{\pi} \right)^3 \left( 190.4 - 26.66 n_l + 0.6527 n_l^2 \right). \tag{37}
\end{align*}
\]

The numbers displayed in Eq. (37) have been taken from Ref. [12]. The light quark mass corrections in the linear approximation read

\[
\begin{align*}
\delta^{(2)}_{\text{massive}} &= \frac{\bar{a}_s^2}{6} \overline{\text{M}}_Q(\overline{\text{M}}_Q), \tag{38} \\
\delta^{(3)}_{\text{massive}} &= \frac{\bar{a}_s^2}{12} \left( \frac{\bar{a}_s}{\pi} \right) \overline{\text{M}}_Q \left[ \beta_0 \left( \ln \frac{\overline{\text{M}}_Q^2}{m^2} - 4 \ln 2 + \frac{14}{3} \right) \\
&+ \frac{4}{3} \left( \frac{59}{15} + 2 \ln 2 \right) + \frac{76}{3 \pi} \left( c_1 c_2 + d_1 d_2 \right) \right]. \tag{39}
\end{align*}
\]

If the \(\overline{\text{MS}}\) definition is used for the charm quark mass, \(m = \overline{\text{m}}(\overline{\text{m}})[1 + \frac{4}{3}(\bar{a}_s/\pi)]\), we have to apply the replacement

\[
\delta^{(2)}_{\text{massive}}(m, \overline{\text{M}}_Q(\overline{\text{M}}_Q), \bar{a}_s) \rightarrow \delta^{(2)}_{\text{massive}}(\overline{\text{m}}(\overline{\text{m}}), \overline{\text{M}}_Q(\overline{\text{M}}_Q), \bar{a}_s) + \epsilon \delta^{(1)}(\bar{a}_s) \delta^{(2)}_{\text{massive}}(m, \overline{\text{M}}_Q(\overline{\text{M}}_Q), \bar{a}_s) + \ldots \]  \tag{40}
\]

in Eq. (34). The generalization to the case where more than one of the light quarks has a finite mass is straightforward. The parameter \(\epsilon (\epsilon = 1)\) is an auxiliary variable that facilitates the determination

\(^6\)The relation between perturbative orders (LO, NLO, etc.) in the non-relativistic power-counting scheme and perturbative orders \((\alpha_s, \alpha_s^2, \text{etc.}, \text{or one-loop, two-loop, etc.})\) in quantities unrelated to non-relativistic quark–antiquark physics, such as the pole–\(\overline{\text{MS}}\) mass relation, can also be seen from Eqs. (31) and (33). The order \(\alpha_s^2\) linear light quark mass term is obtained from the static potential at NLO, the order \(\alpha_s^3\) linear light quark mass term is obtained from the static potential at NNLO, etc.
of the heavy quark $\overline{\text{MS}}$–1S mass relation in Sec. 5, where the non-relativistic power counting and the ordinary power counting via the number of loops have to be combined in such a way that the linear sensitive contributions cancel systematically in each order. Equation (34) is the basic equation that we will use for the determination of the bottom $\overline{\text{MS}}$ mass in this work. For the corrections coming from the charm quark mass, we will only use the linear mass approximation. We show in this section that this approximation should be sufficient to give a description of the charm mass effects with a relative uncertainty of 10%. We also demonstrate that the linear mass approximation becomes better at higher orders by explicitly comparing the linear mass terms with known exact results.

At order $\alpha_s^2$ the light quark mass corrections can be represented as an integral over the one-loop gluon virtuality times the subtracted light quark vacuum polarization $P$ [34], in analogy to the NLO light quark mass corrections to the static potential in Eq. (13) ($r = m/M_Q$):

$$
\delta^{(2),\text{full massive}} = \frac{4}{3} \left( \frac{\alpha_s}{\pi} \right)^2 \frac{1}{24} \int_0^\infty dq^2 \left[ \frac{1}{2} \frac{q^2}{M_Q^2} \left( 1 - \frac{1}{2} \frac{q^2}{M_Q^2} \right) \left( 1 + 4 \frac{M_Q^2}{q^2} \right)^{3/2} \right] P \left( \frac{m^2}{q^2} \right)
$$

$$
= \frac{4}{3} \left( \frac{\alpha_s}{\pi} \right)^2 \frac{1}{4} \left[ \ln^2(r) + \frac{\pi^2}{6} \left( \ln(r) + \frac{3}{2} \right) r^2 
+ (1 + r) (1 + r^3) \left( \text{Li}_2(-r) - \frac{1}{2} \ln^2(r) + \ln(r) \ln(1 + r) + \frac{\pi^2}{6} \right) 
+ (1 - r) (1 - r^3) \left( \text{Li}_2(r) - \frac{1}{2} \ln^2(r) + \ln(r) \ln(1 - r) - \frac{\pi^2}{3} \right) \right]
$$

$$
= \frac{4}{3} \left( \frac{\alpha_s}{\pi} \right)^2 \left[ \frac{\pi^2}{8} r - 3 \frac{r^2}{4} + \frac{\pi^2}{8} r^3 - \frac{1}{4} \ln^2(r) - \frac{13}{24} \ln(r) + \frac{\pi^2}{24} + \frac{151}{288} \right] r^4 
- \sum_{n=3}^\infty \left( 2 F(n) \ln(r) + F'(n) \right) r^{2n}
$$

(41)

where $P$ is defined in Eq. (15) and

$$
F(n) = \frac{3 (n - 1)}{4 n (n - 2) (2n - 1) (2n - 3)},
$$

(42)

$$
F'(n) = \frac{d}{dn} F(n).
$$

(43)

Equation (41) is ultraviolet-finite owing to the subtraction of the massless vacuum polarization in the function $P$. From the first line of Eq. (41) it is straightforward to see that in the limit $m \ll M_Q$ two momentum regions contribute to the integral: $q \sim m$ and $q \sim M_Q$. Thus, the expansion in terms of $m/M_Q$ cannot be obtained by naively Taylor-expanding the momentum integral in the first line of Eq. (41), since this would only extract the contributions of the high momentum region $q \sim M_Q$. The linear light quark mass term and all the other terms that are non-analytic in $m^2$, such as $m^3$ and $m^{2n} \ln m$, originate from the low momentum region $q \sim m$. To obtain the linear light quark mass term directly, we therefore have to carry out a non-relativistic expansion in $q^2/M_Q^2$:

$$
\delta^{(2),\text{massive}} = \frac{4}{3} \left( \frac{\alpha_s}{\pi} \right)^2 \frac{1}{24} \int_0^\infty dq^2 \left[ \frac{2}{M_Q} \right] P \left( \frac{m^2}{q^2} \right)
$$

(44)

16
\[
\frac{\delta (2)}{\text{massive}} / \left( \frac{1}{4} \frac{(a_s)^2}{\pi} \right) = 0.123, 0.247, 0.370, 0.493, 0.617
\]

\[
\frac{\delta (2)}{\text{massive}} / \delta_{\text{full}}^{(2)} = 1.06, 1.11, 1.16, 1.20, 1.24
\]

Table 1: Comparison of the full result (second line) and the linear mass approximation (third line) for the order \( \alpha_s^2 \) light quark mass corrections in the heavy quark pole-\( \overline{\text{MS}} \) mass relation for various values of the ratio \( m/M_Q \). The ratio of linear mass approximation to full result is shown in the fourth line.

\[
\delta_{\text{massive}}^{(3), \text{vac, full}} = \frac{1}{6} a_s^2 \frac{m}{M_Q}
\]

We emphasize that the light quark vacuum polarization has to be fully taken into account without any expansion. Comparing Eq. (44) with Eq. (18), we also see the equality to \( -1/2 \) of the static potential at zero distance, Eq. (33). This explicitly demonstrates the cancellation of the linear light quark mass terms in the total static energy (32) at order \( \alpha_s^2 \) for the case where the expansion in \( m \) is allowed. In Table 1 the size of the order \( \alpha_s^2 \) light quark mass corrections is displayed for the full result and the linear mass approximation for \( m/M_Q \) between 0.1 and 0.5. The ratio of the light quark mass terms versus the full result is also shown. For \( m/M_Q = 0.3 \) (0.5) the linear mass terms account for 116% (124%) of the full result. We see that the linear mass approximation is remarkably good, even for rather large values of \( m/M_Q \), owing to the \( \pi^2 \) enhancement factor.

As already mentioned before, the full form of the order \( \alpha_s^3 \) light quark mass corrections is not yet known. However, we can compare the full result and the linear mass approximation for the corrections that can be obtained from insertions of one-loop light quark vacuum polarizations into the one-loop gluon line. For illustration, in Eq. (22) the light quark mass corrections that can be obtained from insertions of one-loop light quark vacuum polarizations correspond to the terms that involve the function \( P \). (In \( \delta_{\text{massive}}^{(3)} \), Eq. (39), the order \( \alpha_s^3 \) linear light quark mass corrections that can be obtained from one-loop light quark vacuum polarization insertions correspond to the terms that remain after setting \( c_1 = c_2 = d_1 = d_2 = 0 \).) In the relation between the heavy quark pole and the \( \overline{\text{MS}} \) mass, the light quark mass vacuum polarization corrections at order \( \alpha_s^3 \) read

\[
\delta_{\text{massive}}^{(3), \text{vac, full}} = \frac{4}{3} a_s^3 \frac{1}{\pi} \frac{1}{48} \int_0^{\infty} dq^2 \frac{q^2}{M_Q^2} \left[ \frac{1}{2} P^2 \left( \frac{m^2}{q^2} \right) \left( 1 + \frac{4}{M_Q^2} \right) - \beta_0 \ln \left( \frac{q^2}{\mu^2} \right) + a_1 \right]
\]

\[
\times \left[ P^2 \left( \frac{m^2}{q^2} \right) - \beta_0 \ln \left( \frac{q^2}{\mu^2} \right) + a_1 \right] + \frac{1}{3} P^2 \left( \frac{m^2}{q^2} \right)
\]

\[
= \frac{4}{3} a_s^3 \frac{1}{12} \left[ \beta_0 \left( \ln \left( \frac{\mu^2}{M_Q^2} \right) f^{(0)}_P \left( \frac{m}{M_Q} \right) - f^{(1)}_P \left( \frac{m}{M_Q} \right) \right) + a_1 f^{(0)}_P \left( \frac{m}{M_Q} \right) + \frac{1}{3} f^{(0)}_P \left( \frac{m}{M_Q} \right) \right],
\]
Table 2: Comparison of the full result (second line) and the linear mass approximation (third line) for the order $\alpha_s^3$ light quark mass corrections in the heavy quark pole–$\overline{\text{MS}}$ mass relation for $\mu = m$, for various values of the ratio $m/M_Q$. The ratio of linear mass approximation to full result is shown in the fourth line.

<table>
<thead>
<tr>
<th>$m/M_Q$</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta^{(3)}_{\text{vac,full}}/\left(\frac{3}{4}\left(\frac{a_s^2}{\pi}\right)^3\right)$</td>
<td>0.689</td>
<td>1.521</td>
<td>2.419</td>
<td>3.352</td>
<td>4.305</td>
</tr>
<tr>
<td>$\delta^{(3)}_{\text{mass,full}}/\left(\frac{3}{4}\left(\frac{a_s^2}{\pi}\right)^3\right)$</td>
<td>0.536</td>
<td>1.072</td>
<td>1.608</td>
<td>2.144</td>
<td>2.681</td>
</tr>
<tr>
<td>$\delta^{(3)}<em>{\text{vac,linear}}/\delta^{(3)}</em>{\text{mass,linear}}$</td>
<td>0.78</td>
<td>0.71</td>
<td>0.67</td>
<td>0.64</td>
<td>0.62</td>
</tr>
</tbody>
</table>

Fully analytic results for $f_P^{(0)}$, $f_P^{(1)}$, and $f_{PP}^{(0)}$ can be found in App. D. In Table 2 the size of the order $\alpha_s^3$ light quark vacuum polarization corrections is displayed for the full result and for the linear mass approximation, for $m/M_Q$ between 0.1 and 0.5 and $\mu = m$. The ratio of the linear approximation to the full result is also shown. From the first line of Eq. (46), it is clear why one expects the linear mass approximation to become better at higher orders: higher orders of perturbation theory correspond to either larger powers of the subtracted vacuum polarization function $P$, or to larger powers of $\ln q^2$. Both enhance the contributions coming from the low momentum region $q \sim m$ with respect to the contributions from $q \sim M_Q$. We note that higher powers of $P$ are not suppressed for small $q$ due to the subtraction of the massless vacuum polarization, see Eq. (15). However, the numbers in Table 2 show that, in contrast to this argument, the linear mass approximation for the order $\alpha_s^3$ vacuum polarization contributions is in fact much worse than for the order $\alpha_s^2$ light quark mass corrections. For $m/M_Q = 0.3$ (0.5) the linear mass terms only account for 67% (62%) of the complete result. Having a closer look at the second line of Eq. (46), however, one finds that this behaviour is caused by a cancellation between $f_P^{(0)}$ and $f_P^{(1)}$, and the fact that the corrections to their linear mass approximations have a different
Table 3: The functions $f_P^{(n)}$ and $f_{PP}^{(n)}$, which describe the corrections coming from light quark vacuum polarization insertions into the one-loop gluon line of the heavy quark pole–$\overline{\text{MS}}$ mass relation, for various values of $n$ and for $m/\overline{M}_Q = 0.3$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[f_P^{(n)}]_{\text{lin}}/f_P^{(n)}$</td>
<td>1.17</td>
<td>0.88</td>
<td>1.10</td>
<td>0.92</td>
<td>1.07</td>
<td>0.94</td>
<td>1.05</td>
<td>0.96</td>
<td>1.04</td>
<td>0.97</td>
<td>1.03</td>
</tr>
<tr>
<td>$[f_{PP}^{(n)}]<em>{\text{lin}}/f</em>{PP}^{(n)}$</td>
<td>1.016</td>
<td>1.003</td>
<td>1.001</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
</tbody>
</table>

Table 4: Comparison of the full result (second line) and the linear mass approximation (third line) for the sum of the order $\alpha_s^2$ and $\alpha_s^3$ light quark mass corrections in the bottom quark pole–$\overline{\text{MS}}$ mass relation for $m = 1.5$ GeV, $\overline{M}_Q = 4.2$ GeV and $\alpha_s^{(5)}(M_Z) = 0.118$, for various values of the renormalization scale $\mu$. The ratio of linear mass approximation to full result is shown in the fourth line.

<table>
<thead>
<tr>
<th>$\mu/\text{[GeV]}$</th>
<th>1.0</th>
<th>1.5</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>3.5</th>
<th>4.0</th>
<th>4.5</th>
<th>5.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta^{(2),\text{full}}<em>{\text{massive}} + \delta^{(3),\text{vac,full}}</em>{\text{massive}}$</td>
<td>0.0750</td>
<td>0.0488</td>
<td>0.0333</td>
<td>0.0324</td>
<td>0.0286</td>
<td>0.0259</td>
<td>0.0239</td>
<td>0.0223</td>
<td>0.0210</td>
</tr>
<tr>
<td>$\delta^{(2)}<em>{\text{massive}} + \delta^{(3),\text{vac}}</em>{\text{massive}}$</td>
<td>0.0607</td>
<td>0.0455</td>
<td>0.0375</td>
<td>0.0325</td>
<td>0.0292</td>
<td>0.0268</td>
<td>0.0249</td>
<td>0.0234</td>
<td>0.0222</td>
</tr>
<tr>
<td>linear app./full</td>
<td>0.81</td>
<td>0.93</td>
<td>0.98</td>
<td>1.00</td>
<td>1.02</td>
<td>1.03</td>
<td>1.04</td>
<td>1.05</td>
<td>1.05</td>
</tr>
</tbody>
</table>

Despite the rather good approximation provided by the linear mass terms at large orders, the fact remains that they only account for about 70% of the order $\alpha_s^3$ light quark mass corrections, for values of $m/\overline{M}_Q$ that are relevant to the charm mass effects in the bottom pole–$\overline{\text{MS}}$ mass relation. At this point it is instructive to compare the sum of the order $\alpha_s^2$ light quark mass corrections and the order $\alpha_s^3$ light quark mass vacuum polarization corrections displayed in Eqs. (41) and (46), $\delta^{(2),\text{full}}_{\text{massive}} + \delta^{(3),\text{vac,full}}_{\text{massive}}$, with the corresponding linear mass approximation of the sum, $\delta^{(2)}_{\text{massive}} + \delta^{(3),\text{vac}}_{\text{massive}}$. Table 4 shows the full result (second line), the linear mass approximation (third line) and the ratio (fourth line) for $m = 1.5$ GeV, $\overline{M}_b = 4.2$, $\alpha_s^{(n=4)}(M_Z) = 0.118$ and $\mu = 1–5$ GeV, where $\mu$ is the scale used in the strong coupling. For the strong coupling we used four-loop running [36] and three-loop matching conditions [37] at the five-four quark flavour threshold at $\mu = \overline{M}_b$. It is an interesting observation that, although the linear approximation differs from the full result by +18% at order $\alpha_s^2$ and −35% at order $\alpha_s^3$ (at $\mu = m$), the difference amounts to only −7% for the sum. Therefore, instead of using the full result at order $\alpha_s^2$ and the linear mass approximation at order $\alpha_s^3$, it seems more advantageous to employ the linear mass approximation at order $\alpha_s^2$ and $\alpha_s^3$.

[We remind the reader that the order $\alpha_s^3$ terms are as large as the order $\alpha_s^2$ ones, see Sec. 2.3.] This is the reason why, in this work, we will employ only the linear approximation for the charm quark mass corrections in the bottom pole–$\overline{\text{MS}}$ mass relation, as displayed in Eq. (34). We emphasize that this decision is
only based on the examination of the order $\alpha_s^3$ light quark mass corrections coming from vacuum polarization insertions. They account for about 40% ($\mu = m$) to 70% ($\mu = 3m$) of the full result in the linear mass approximation. A calculation of the full order $\alpha_s^3$ light quark mass corrections would be useful to remove this source of uncertainty for the charm mass corrections determined in this work.

4 Light Quark Mass Corrections in the Heavy Quark Pole–1S Mass Relation

The heavy quark pole mass is quite a convenient parameter to carry out bound state calculations because, in the pole mass scheme, the Schrödinger equation, which describes the non-relativistic dynamics of a perturbative heavy-quark–antiquark pair at NNLO, has the simple form shown in Eq. (1). However, as has been noted before, the heavy quark pole mass parameter should not be employed in an actual analysis for the numerical determination of the heavy quark mass. In practice, in the pole mass scheme, the determination of the heavy quark mass parameter is spoiled by a large correlation to the value of the strong coupling, large perturbative corrections and large renormalization scale variations. Thus it is advantageous to keep the pole mass parameters for the actual bound state calculations, but to eliminate it later in favour of a better defined mass with a reduced sensitivity to small momenta and without an ambiguity of order $\Lambda_{\text{QCD}}$. Such mass definitions are called “short-distance masses”. The well-known $\overline{\text{MS}}$ mass definition is the prototype of a short-distance mass. However, for the description of the heavy-quark–antiquark bound state dynamics through Eq. (1), the $\overline{\text{MS}}$ mass definition turns out to be a rather bad choice because it breaks the non-relativistic power counting. This breakdown can be visualized in Eq. (1): after eliminating the heavy quark pole mass in favour of the $\overline{\text{MS}}$ mass

$$M_Q^{\text{pole}} \rightarrow \overline{M}_Q(\overline{M}_Q) + \frac{4}{3} \left( \frac{\alpha_s}{\pi} \right) \overline{M}_Q(\overline{M}_Q) + \ldots,$$

the additional correction terms coming from the external energy term $E = \sqrt{s} - 2M_Q^{\text{pole}}$ dominate all other terms, which are proportional to $\alpha_s^2$ and higher powers of $\alpha_s$. In practice, if we extract the heavy quark $\overline{\text{MS}}$ mass with this method, while taking care of the proper cancellation of the contributions that are linearly sensitive to small momenta, the results have a large correlation with the choice of the strong coupling and a large renormalization scale dependence, which is comparable to the pole mass case. (See Ref. [38] for a comparison of the heavy quark pole, $\overline{\text{MS}}$ and 1S mass definition in the framework of bottom and top mass determinations from bound state calculations.) From the conceptual point of view the heavy quark $\overline{\text{MS}}$ is not suited to the quark–antiquark bound state problem, because it is a short-distance mass genuinely designed for processes where the heavy quark is very off-shell. This means that it is a good choice for high energy processes (such as heavy quark production at high energies), or for processes where the external energies are much smaller than the heavy quark mass (such as virtual heavy quark corrections in low energy processes). A short-distance mass definition that is suited to processes where the heavy quark is very close to its mass-shell (i.e. for situations where $q^2 - M_Q^2 \ll M_Q^2$) is the 1S mass. The 1S mass was introduced in Refs. [9, 39] to address the previously mentioned issues for bottom and top quark mass extractions from the $\Upsilon$ sum rules and from top–antitop quark pair production close to threshold at a future Linear Collider. Other heavy quark
mass definitions with similar properties were proposed in Ref. [40] (kinetic mass) and in Ref. [31] (PS mass).

The heavy quark 1S mass is defined as half of the perturbative contribution to the mass of a \( J^{PC} = 1^{--} \), \( ^3S_1 \) quark–antiquark bound state, assuming that the heavy quark is stable. In the case of the bottom quark, it corresponds to half of the perturbative contributions of the mass of the \( \Upsilon(1S) \) meson. We emphasize that the 1S mass is a priori a purely formal parameter. Its relation to the heavy quark pole mass, and any other mass definition that is defined perturbatively, is determined using the non-relativistic power counting for perturbative heavy-quark–antiquark systems (i.e. assuming that the scale hierarchy \( M_Q \gg M_Q v \gg M_Q v^2 \gg \Lambda_{QCD} \) is realized) regardless, whether this assumption is valid in reality or not. For the top–antitop quark system it is certainly valid in most cases, for the bottom–antibottom quark system it is debatable for low radial excitations, whereas for the charm–anticharm system it is definitely not valid at all. Nevertheless, the 1S mass could be employed in all cases through its perturbative relation to other mass definitions. However, the 1S mass is most useful for systems that are truly perturbative, because for these systems it has a direct physical interpretation as representing the perturbative contribution of the mass of the \( J^{PC} = 1^{--} \), \( ^3S_1 \) heavy quarkonium ground state.

In this section we present the NNLO light quark mass corrections to the relation between the heavy quark 1S and pole masses. As in the previous section, we will assume that there are \( n_l \) light quark species, of which one has a finite (pole) mass \( m \), and we adopt the convention that the strong coupling evolves with \( n_l \) quark flavours.

### 4.1 Results

The relation between the heavy quark 1S and pole masses at NNLO in the non-relativistic expansion including the light quark mass corrections can be parametrized as \( (a_s = \alpha_s^{(n_l)}(\mu)) \):

\[
M_1^{1S} = M_\text{pole}^Q \left\{ 1 - \epsilon \left[ \Delta^\text{LO}(a_s) \right] - \epsilon^2 \left[ \Delta^\text{NLO}_{\text{massless}}(M_1^{\text{pole}}, a_s, \mu) + \Delta^\text{NLO}_{\text{massive}}(m, M_\text{pole}^Q, a_s) \right] 
\right. 
\left. - \epsilon^3 \left[ \Delta^\text{NNLO}_{\text{massless}}(M_1^{\text{pole}}, a_s, \mu) + \Delta^\text{NNLO}_{\text{massive}}(m, M_\text{pole}^Q, a_s, \mu) \right] \right\} ,
\]  

(53)

where the subscript “massless” indicates the corrections for massless light quarks and the subscript “massive” the corrections from the light quark mass. The massless corrections are well known and read

\[
\Delta^\text{LO} = \frac{C_F^2 a_s^2}{8},
\]

(54)

\[
\Delta^\text{NLO}_{\text{massless}} = \frac{C_F^2 a_s^2}{8} \left( \frac{a_s}{\pi} \right) \left[ \beta_0 \left( L + 1 \right) + \frac{a_1}{2} \right],
\]

(55)

\[
\Delta^\text{NNLO}_{\text{massless}} = \frac{C_F^2 a_s^2}{8} \left( \frac{a_s}{\pi} \right)^2 \left[ \beta_0^2 \left( \frac{3}{4} L^2 + \frac{3}{2} + \frac{\zeta_3}{2} + \frac{\pi^2}{24} + \frac{1}{4} \right) + \beta_0 a_1 \left( \frac{3}{2} L + 1 \right) \right. 
\left. + \frac{\beta_4}{4} \left( L + 1 \right) + \frac{a_1^2}{16} + \frac{a_2}{8} + \left( C_A - \frac{C_F}{48} \right) C_F \pi^2 \right],
\]

(56)
where

\[ L \equiv \ln \left( \frac{\mu}{C_F a_s M_{\text{pole}}^2} \right). \] 

(57)

The one- and two-loop coefficients of the beta-function, \( \beta_0 \) and \( \beta_1 \), and the constants \( a_1 \) and \( a_2 \) are given in Eqs. (7)–(10). The NNLO corrections for massless light quarks were first calculated in Ref. [3]. The contributions at LO, NLO and NNLO have been labelled by powers of \( \epsilon, \epsilon^2 \) and \( \epsilon^3 \), respectively, of the auxiliary parameter \( \epsilon = 1 \), that has already been employed for Eq. (34) and that will be relevant in Sec. 5 when we determine the relation between the heavy quark \( \overline{MS} \) and 1S masses. The results at NLO and NNLO are obtained by starting from the known S-wave ground state solution \((r = |r|)\),

\[ \phi_{1S}(r) = \langle r | 1S \rangle = \langle 1S | r \rangle = \pi^{-\frac{1}{2}} \frac{\epsilon}{2} e^{-\gamma r}, \] 

(58)

\[ \gamma = \frac{M_{\text{pole}}^2 C_F a_s}{2}, \] 

(59)
of the LO Schrödinger equation,

\[ \left( -\nabla^2 + V_{\text{LO}}(r) - 2 M_{\text{pole}}^2 \Delta_{\text{LO}} \right) \phi_{1S}(r) = 0, \] 

(60)

and by using Rayleigh–Schrödinger time-independent perturbation theory to calculate the higher order corrections. The formal results for the light quark mass corrections at NLO and NNLO can be quickly written down using the Dirac notation:

\[ -2 M_{\text{Q}}^2 \Delta_{\text{NLO massive}} = \langle 1S | \delta V_{\text{NLO massive}} | 1S \rangle, \] 

(61)

\[ -2 M_{\text{Q}}^2 \Delta_{\text{NLO massive}} = \langle 1S | \delta V_{\text{NLO massive}} | 1S \rangle + \sum_{i \neq 1S} \frac{\langle 1S | \delta V_{\text{NLO massless}} | i \rangle \langle i | \delta V_{\text{NLO massless}} | 1S \rangle}{E_{1S} - E_i}, \] 

(62)

where \( V_{\text{NLO massless}}(r) \), \( \delta V_{\text{NLO massive}}(r) \), and \( \delta V_{\text{NLO massless}}(r) \) are given in Eqs. (3), (18) and (30), respectively. Details of the calculations required by Eqs. (61) and (62) are presented in App. A. The final results for \( \Delta_{\text{NLO massive}} \) and \( \Delta_{\text{NNLO massive}} \) read \((a_s = \alpha_s^{(n)}(\mu))\)

\[ \Delta_{\text{NLO massive}} = \frac{C_F^2 a_s^2}{4} \left( \frac{a_s}{3 \pi} \right) \left\{ h_0(a) + \ln \left( \frac{a}{2} \right) + \frac{11}{6} \right\}, \] 

(63)

\[ \Delta_{\text{NNLO massive}} = \frac{C_F^2 a_s^2}{4} \left( \frac{a_s}{3 \pi} \right)^2 \left\{ 3 \beta_0 \left[ \frac{3}{2} \left( \ln \left( \frac{a}{2} \right) + h_0(a) - \frac{1}{3} \tilde{h}_0(a) + \frac{3}{2} \right) \ln \left( \frac{\mu}{2 \gamma} \right) + \frac{5}{6} \right] + \ln \left( \frac{a}{2} \right) - \frac{1}{2} \tilde{h}_0(a) - h_1(a) - h_7(a) + \zeta_3 + \frac{\pi^2}{12} + \frac{4}{3} \right\} + \frac{3}{2} \ln \left( \frac{a}{2} \right) \left( \ln \left( \frac{a}{2} \right) + 2 h_0(a) - \frac{2}{3} \tilde{h}_0(a) - 9 \right), \]
\[
\frac{1}{2} h_0(a) \left( h_0(a) - 2 \tilde{h}_0(a) + 4 h_4(a) - 31 \right) \\
+ \frac{25}{6} \tilde{h}_0(a) - 2 h_1(a) - h_2(a) + h_5(a) - 2 h_7(a) + \zeta_3 + \frac{\pi^2}{12} - \frac{571}{24} \\
\frac{57}{4} \left( c_1 c_2 a + \frac{d_1 d_2 a}{1 + d_2 a} + c_1 \ln(1 + c_2 a) + d_1 \ln(1 + d_2 a) \right), \tag{64}
\]

where

\[
a \equiv \frac{m}{\gamma} = \frac{2 m}{C_F a_s M_{\text{pole}}^2}, \tag{65}
\]

and

\[
h_0(a) \equiv \int_1^\infty dx \frac{f(x)}{(1 + a x)^2} = -\frac{11}{6} + \frac{3\pi}{4} a - 2 a^2 + \pi a^3 + \frac{2 - a^2 - 4 a^4}{\sqrt{a^2 - 1}} \arctan \left( \frac{\sqrt{a - 1}}{\sqrt{a + 1}} \right), \tag{66}
\]

\[
\tilde{h}_0(a) \equiv a \frac{d}{da} h(a) = 2 \left( h_3(a) - h_0(a) \right) = \frac{2 + 7 a^2 - 12 a^4}{2(a^2 - 1)} + \frac{3\pi}{4} (1 + 4 a^2) a - \frac{3 a^4 (4 a^2 - 5)}{(a^2 - 1)^{\frac{3}{2}}} \arctan \left( \frac{\sqrt{a - 1}}{\sqrt{a + 1}} \right), \tag{67}
\]

\[
h_1(a) \equiv \int_1^\infty dx \frac{f(x)}{a^2 x^2 - 1} \left( 1 - \frac{2 a x}{a^2 x^2 - 1} \ln(a x) \right), \tag{68}
\]

\[
h_2(a) \equiv \int_1^\infty dx \frac{f(x)}{(1 + a x)^2} \left[ \frac{5}{3} + \frac{1}{x^2} \left( 1 + \frac{1}{2 x} \sqrt{x^2 - 1} \ln \left( \frac{x - \sqrt{x^2 - 1}}{x + \sqrt{x^2 - 1}} \right) \right) \right], \tag{69}
\]

\[
h_3(a) \equiv \int_1^\infty dx \frac{f(x)}{(1 + a x)^3} = \frac{28 + 23 a^2 - 60 a^4}{12 (a^2 - 1)} + \frac{\pi}{8} (9 + 20 a^2) a - \frac{4 - 6 a^2 - 21 a^4 + 20 a^6}{2 (a^2 - 1)^{\frac{3}{2}}} \arctan \left( \frac{\sqrt{a - 1}}{\sqrt{a + 1}} \right), \tag{70}
\]

\[
h_4(a) \equiv \int_1^\infty dx \frac{f(x)}{(1 + a x)^2} \ln(1 + a x), \tag{71}
\]

\[
h_5(a) \equiv \int_1^\infty dx \int_1^\infty dy \frac{f(x) f(y)}{(1 + a x)^2 (1 + a y)^2} \frac{a^2 x y}{1 + a (x + y)}, \tag{72}
\]

\[
h_6(a) \equiv \int_1^\infty dx \int_1^\infty dy \frac{f(x) f(y)}{(1 + a x)^2 (1 + a y)^2} \ln \left( 1 + a (x + y) \right), \tag{73}
\]

23
\[ h_f(a) \equiv \int_1^\infty dx \frac{f(x)}{(1 + a x)^2} \text{Li}_2\left( \frac{a x}{1 + a x} \right). \]  

(74)

The function \( f \) is defined in Eq. (17). It is instructive to consider the limit \( m \ll M_Q \alpha_s \) of Eqs. (63) and (64),

\[-2 M_Q^\text{pole} \Delta^{NLO}_\text{massive} \xrightarrow{m \ll M_Q \alpha_s} -2 C_F \left( \frac{a_s}{\pi} \right)^2 \frac{\pi^2}{8} m + 2 C_F \left( \frac{a_s}{\pi} \right) \frac{9}{16} \frac{m^2}{M_Q^\text{pole}} + \mathcal{O}\left( a_s^2 \frac{m^3}{(M_Q a_s)^2} \right), \]  

(75)

\[-2 M_Q^\text{pole} \Delta^{NNLO}_\text{massive} \xrightarrow{m \ll M_Q \alpha_s} -2 C_F \left( \frac{a_s}{\pi} \right)^3 \frac{\pi^2}{16} m \left[ \beta_0 \left( \ln \frac{\mu^2}{m^2} - 4 \ln 2 + \frac{14}{3} \right) - \frac{4}{3} \left( \frac{59}{15} + 2 \ln 2 \right) + \frac{76}{3\pi} \left( c_1 c_2 + d_1 d_2 \right) \right] + \mathcal{O}\left( a_s^2 \frac{m^2}{M_Q a_s} \right). \]  

(76)

If \( m \approx M_Q \alpha_s \), as is the case for the charm mass effects in the bottom pole–1S mass relation, the expansion in the charm quark mass is completely meaningless as each term in the expansion is of equal size. From Eqs. (75) and (76) we see that the linear light quark mass terms in the static potential are \( r \)-independent and because all LO states form an orthogonal set. Thus, multiple insertions of the static potential at higher orders of Rayleigh–Schrödinger perturbation theory do not lead to any linear light quark mass terms. If the \( \overline{\text{MS}} \) definition is used for the charm quark mass, \( m = \overline{m}(\overline{m})[1 + \frac{Q}{3}(\frac{\alpha_s}{\pi})] \), we have to apply the replacement

\[ \Delta^{NLO}_\text{massive}(m, M_Q^\text{pole}, a_s) \rightarrow \Delta^{NLO}_\text{massive}(\overline{m}(\overline{m}), M_Q^\text{pole}, a_s) + \epsilon \frac{4}{3} \left( \frac{a_s}{\pi} \right) \Delta^{NLO}_\text{massive}(\overline{m}(\overline{m}), M_Q^\text{pole}, a_s) \]  

(77)

in Eq. (53), where

\[ \Delta^{NLO}_\text{massive} = a \frac{d}{da} \Delta^{NLO}_\text{massive} = C_F^2 a_s^2 \left( \frac{a_s}{3\pi} \right) \left\{ \tilde{h}_0(a) + 1 \right\}, \]  

(78)

and \( \tilde{h}_0 \) is defined in Eq. (67).

In order to implement the 1S mass into the moments of the bottom–antibottom cross section for the sum rule analysis we need the inverse of Eq. (53), using the non-relativistic power counting, i.e. with respect to the non-relativistic expansion in \( \alpha_s \) (and not in \( \epsilon \)). The result reads

\[ M_Q^\text{pole} = M_Q^{1S} \left\{ 1 + \Delta^{LO}(a_s) + \left[ \Delta^{NLO}_\text{massless}(M_Q^{1S}, a_s, \mu) + \Delta^{NLO}_\text{massive}(m, M_Q^{1S}, a_s) \right] \right. \]

\[ + \left[ \left( \Delta^{LO}(a_s) \right)^2 + \Delta^{NNLO}_\text{massless}(M_Q^{1S}, a_s, \mu) + \Delta^{NNLO}_\text{massive}(m, M_Q^{1S}, a_s, \mu) \right] \right\}. \]  

(79)

4.2 Double Insertion of the NLO Static Potential

We already mentioned after Eq. (76) that in the limit \( m \to 0 \) the linear light quark mass terms in \( \Delta^{NNLO}_\text{massive} \) only arise from the single insertion of the NNLO light quark mass corrections to the static potential (first term on the RHS of Eq. (62)). This means that—if one is allowed to make the expansion in the light quark mass—the light quark mass corrections coming from multiple insertions
are subleading with respect to those arising from single insertions. For the charm mass corrections, however, an expansion in the charm mass is a priori not possible because $\langle 1/r \rangle \sim M_{c}\alpha_s \sim m_{charm}$. Thus one can not necessarily argue that charm mass corrections arising from multiple insertions are smaller than single insertion ones, at least in low orders of perturbation theory. In high orders of perturbation theory, on the other hand, charm mass corrections coming from multiple insertions are subleading because, as already mentioned, the contributions from small momenta enhance the linear mass terms with respect to higher powers of the charm mass.

In this section we examine the size of the NNLO charm mass corrections in the bottom 1S mass, $\Delta_{\text{massive}}^{\text{NNLO}}$, coming from double insertions of the NLO static potential (second and third terms on the RHS of Eq. (62)). This will be important for the calculation of the NNLO charm mass corrections to the sum rules in Sec. 6, where we neglect the double insertion contributions. From the results given in App. A, the NNLO light quark mass corrections coming from double insertions read

$$\Delta_{\text{massive},d}^{\text{NNLO}} = -\frac{C_F}{4} \frac{\alpha_s^2}{(3\pi)^2} \left\{ \frac{3}{2} \beta_0 \left[ h_0(a) \left( 3 \ln \left( \frac{2\gamma}{\mu} \right) - 2 \right) + 2 h_3(a) \left( 1 - \ln \left( \frac{2\gamma}{\mu} \right) \right) + 2 h_7(a) \right] \right.$$  
$$\left. + \left( \ln \left( \frac{a}{2} \right) + \frac{5}{6} \right) \ln \left( \frac{2\gamma}{\mu} \right) - 2 \zeta_3 + \frac{\pi^2}{3} - 1 \right\}$$

$$+ \frac{3}{2} a_1 \left[ -\frac{3}{2} h_0(a) + h_3(a) - \frac{1}{2} \ln \left( \frac{a}{2} \right) - \frac{5}{12} \right]$$

$$+ h_0(a) \left( -\frac{5}{2} h_0(a) + 2 h_3(a) - 2 h_4(a) \right) - h_5(a) + h_6(a)$$

$$- 3 h_0(a) \left( \ln \left( \frac{a}{2} \right) + \frac{3}{2} \right) + 2 h_7(a) + 2 h_3(a) \left( \ln \left( \frac{a}{2} \right) + \frac{11}{6} \right)$$

$$- \frac{1}{2} \ln^2 \left( \frac{a}{2} \right) - \frac{5}{6} \ln \left( \frac{a}{2} \right) - \zeta_3 + \frac{\pi^2}{6} - \frac{61}{72} \right\}.$$  \hspace{1cm} (80)

In Fig. 2 we have displayed the ratio $\Delta_{\text{massive},d}^{\text{NNLO}} / \Delta_{\text{massive}}^{\text{NNLO}}$ for $M_{b}^{\text{pole}} = 4.8$ GeV, $\alpha_s^{(5)}(M_{Z}) = 0.118$ and $1$ GeV $\leq \mu \leq 5$ GeV for $m = 0.1$ GeV (dotted line), 0.5 GeV (dash-dotted line), 1.0 GeV (dashed line), 1.5 GeV (long-dash-dotted line) and 2.0 GeV (solid line). For the charm case ($m \approx 1.5$ GeV) we see that the double-insertion contributions amount to about 1% for $\mu \approx 1.5$ GeV and increase to about 10% for $\mu \approx 5$ GeV. This shows that the NNLO corrections already are considerably influenced by momenta smaller than $\langle 1/r \rangle \sim M_{c}\alpha_s$ and that the single-insertion contributions give the dominant contributions to the NNLO light quark mass corrections even for the charm quark case. Thus, in view of the fact that the use of the linear mass approximation for the charm mass corrections in the bottom pole–MS mass relation introduces a relative uncertainty of around 10% in the charm mass corrections, it would be consistent to neglect all double insertions at the NNLO level. This is useful because the calculation of the double insertions is considerably more time-consuming than that of the single insertions. For this reason we believe that it is save, at the level of 10% accuracy for the charm mass corrections, to neglect the double-insertion contributions for the NNLO charm mass corrections to the moments of the $\Upsilon$ sum rules.
Figure 2: The ratio of the double-insertion contributions to the full result for the NNLO light quark mass corrections in the bottom quark 1S–pole mass relation, $\Delta_{\text{massive},d}^{\text{NNLO}} / \Delta_{\text{massive}}^{\text{NNLO}}$ for $M_{Q}^{\text{pole}} = 4.8$ GeV, $\alpha_{s}^{(5)}(M_{Z}) = 0.118$ and $m = 0.1$ GeV (dotted line), 0.5 GeV (dash-dotted line), 1.0 GeV (dashed line), 1.5 GeV (long-dash-dotted line) and 2.0 GeV (solid line) plotted over the renormalization scale $\mu$.

5 Heavy Quark $\overline{\text{MS}}$-1S Mass Relation and Upsilon Expansion

In this work we use the bottom quark 1S mass as the mass definition that is extracted directly from the $\Upsilon$ sum rule analysis. The bottom quark $\overline{\text{MS}}$ mass is then determined in a second step, using Eqs. (34) and (53). However, some care has to be taken in the determination of the perturbative relation between the heavy quark $\overline{\text{MS}}$ and 1S masses to ensure the proper cancellation of the large corrections that are associated with the linear sensitivity to small momenta of the pole mass in Eqs. (34) and (53). Care is needed because Eq. (53), which gives the 1S mass in terms of the pole mass, represents an expansion in the framework of the non-relativistic power counting, where $\alpha_{s} \sim v$. Equation (34), on the other hand, which gives the pole mass in terms of the $\overline{\text{MS}}$ mass, represents a usual Feynman diagram expansion in the number of loops, where the power of $\alpha_{s}$ corresponds to the number of strong coupling constants that occur in the corresponding diagrams. This means that Eqs. (34) and (53) cannot simply be combined by using the expansion in terms of $\alpha_{s}$. Rather, a modified perturbative expansion, the “upsilon expansion” [20], has to be employed. The upsilon expansion gives the following prescription: the LO, NLO and NNLO contributions in Eq. (53) are of order $\epsilon$, $\epsilon^{2}$ and $\epsilon^{3}$, respectively, of the auxiliary parameter $\epsilon = 1$. In Eq. (34), on the other hand, the terms of order $\alpha_{s}^{n}$ are of order $\epsilon^{n}$ in the upsilon expansion. When the $\overline{\text{MS}}$ mass is then expressed in terms of the 1S mass one, must use the expansion in $\epsilon$. This means that, in each order of $\epsilon$, different orders in $\alpha_{s}$ are mixed. This also means that a determination of the heavy quark 1S mass at NNLO in the non-relativistic expansion corresponds to an order $\alpha_{s}^{3}$ determination of the heavy quark $\overline{\text{MS}}$ mass. If the mechanism incorporated in the upsilon expansion is not used, the large corrections mentioned previously can survive and lead to systematic errors. The upsilon expansion prescription can be understood from the asymptotic large
that arises from the contributions that are linearly sensitive to small momenta and that dominate \( c_n \) for large \( n \). This relation comes from the fact that terms that are linearly sensitive to small momenta in \( c_n \) involve powers of the logarithmic term \( L = \ln(\mu/C_F\alpha_s M_Q) \), which exponentiate at higher orders, \( \sum_{i=0}^{\infty} L^i/i! \approx \exp(L) = \mu/C_F\alpha_s M_Q \), and effectively cancel one power of \( \alpha_s \) [20]. Another way to visualize the mechanism behind the upsilon expansion is provided by the light quark mass corrections themselves, as they provide a natural probe for the linear sensitivity to small momenta: the linear light quark mass terms in \( \Delta_{\text{NNLO}} \) and \( \Delta_{\text{NNLO}} \) in Eqs. (75) and (76) are of order \( \alpha_s^2 \) and \( \alpha_s^3 \), respectively; \( \Delta_{\text{NLO}} \) and \( \Delta_{\text{NLO}} \), on the other hand, are of order \( \alpha_s^3 \) and \( \alpha_s^4 \), respectively, in the non-relativistic power counting. The origin of this mismatch is that the non-relativistic dynamics of a perturbative heavy-quark–antiquark system contains scales with powers of \( \alpha_s \) such as the inverse Bohr radius \( M_Q\alpha_s \) as dynamical scales. These scales have to be accounted for by the non-relativistic power counting. The question of sensitivity to small momenta and the corresponding counting of orders, on the other hand, is only relevant to scales that are much smaller than any dynamical one, and therefore not tied to the non-relativistic power counting\(^7\).

5.1 Results

Combining Eqs. (34) and (53) using the upsilon expansion up to order \( \epsilon^3 \) we arrive at the following result for the relation between the heavy quark \( \overline{\text{MS}} \) and the 1S masses (\( \bar{a}_s = \alpha_s^{(\eta)}(M_Q^{1S}) \)),

\[
\overline{M}_Q(M_Q) = M_1^{1S} \left\{ 1 + \epsilon \left[ \Delta^{(1)}(M_1^{1S}, \bar{a}_s) + \Delta^{(2)}(M_1^{1S}, \bar{a}_s) + \Delta^{(3)}(M_1^{1S}, \bar{a}_s) \right] \right\},
\]

where we have separated the corrections for massless light quarks (subscript “massless”) and those coming from the light quark mass (subscript “massive”). Similar to what we did in the previous sections, we consider \( n_l \) light quarks, of which one has a \( \overline{\text{MS}} \) mass \( m_l \). The individual results for the corrections for massless light quarks read

\[
\Delta^{(1)} = \Delta^{\text{LO}} - \delta^{(1)},
\]

\[
\Delta^{(2)} = \Delta^{\text{NLO}} + (\Delta^{\text{LO}})^2 - \delta^{(1)} \Delta^{\text{LO}} - \delta^{(2)} + (\delta^{(1)})^2,
\]

\[
\Delta^{(3)} = \Delta^{\text{NNLO}} + 2 \Delta^{\text{LO}} \Delta^{\text{NLO}} + (\Delta^{\text{LO}})^3 - \left( \frac{\alpha_s}{\pi} \right) \beta_0 (\Delta^{\text{LO}})^2 - \delta^{(1)} \left[ \Delta^{\text{NLO}} + (\Delta^{\text{LO}})^2 \right] - \Delta^{\text{LO}} \left[ \delta^{(2)} - (\delta^{(1)})^2 - \delta^{(3)} + \frac{2\alpha_s}{\beta_0} \right] - \frac{\alpha_s}{\beta_0} \left[ \delta^{(1)} - \Delta^{\text{LO}} \right],
\]

\(^7\)We emphasize that the issue of infrared sensitivity to small momenta, usually also referred to as the “infrared renormalon problem”, is a purely perturbative one. The typical hadronic scale \( \Delta_{\text{QCD}} \) does not arise as a relevant dynamical scale, but only as a dimensionful parameter that parametrizes the renormalon ambiguities in the perturbative series.
where
\[ \Delta^{\text{LO}} \equiv \Delta^{\text{LO}}(\tilde{a}_s), \]  
\[ \Delta^{\text{NLO}} \equiv \Delta^{\text{NLO}}_{\text{massless}}(M_1^{\text{IS}}, \tilde{a}_s, M_Q^{\text{IS}}), \]  
\[ \Delta^{\text{NNLO}} \equiv \Delta^{\text{NNLO}}_{\text{massless}}(M_1^{\text{IS}}, \tilde{a}_s, M_Q^{\text{IS}}), \]  
\[ \delta^{(1)} \equiv \delta^{(1)}(\tilde{a}_s), \]
\[ \delta^{(i)} \equiv \delta^{(i)}_{\text{massless}}(\tilde{a}_s), \quad i = 2, 3. \]  

The formulae for the functions on the RHS of Eqs. (86)–(90) can be found in Eqs. (35)–(37) and (54)–(56). The individual results for the light quark mass corrections read
\[ \Delta_m^{(2)} = \Delta_m^{\text{NLO}} - \delta_m^{(2)}, \]  
\[ \Delta_m^{(3)} = \Delta_m^{\text{NNLO}} + \Delta_m^{\text{NLO}} \left[ 2 \Delta^{\text{LO}} - \delta^{(1)} \right] + \Delta_m^{\text{NLO}} \left[ \delta^{(1)} - \Delta^{\text{LO}} \right] - \delta_m^{(3)}, \]

where
\[ \Delta_m^{\text{NLO}} \equiv \Delta^{\text{NLO}}_{\text{massive}}(\overline{m}(\overline{m}), M_Q^{\text{IS}}, \tilde{a}_s), \]  
\[ \Delta_m^{\text{NNLO}} \equiv \Delta^{\text{NNLO}}_{\text{massive}}(\overline{m}(\overline{m}), M_Q^{\text{IS}}, \tilde{a}_s), \]  
\[ \delta_m^{(2)} \equiv \delta^{(2)}_{\text{massive}}(\overline{m}(\overline{m}), M_Q^{\text{IS}}, \tilde{a}_s), \]
\[ \delta_m^{(3)} \equiv \delta^{(3)}_{\text{massive}}(\overline{m}(\overline{m}), M_Q^{\text{IS}}, \tilde{a}_s). \]

The formulae for the functions on the RHS of Eqs. (93)–(97) can be found in Eqs. (38), (39), (63), (64) and (78). The results for massless light quarks have already been explicitly presented in Ref. [38]. It is worth mentioning that, in the limit \( \overline{m}(\overline{m}) \rightarrow 0 \), \( \Delta_m^{(3)} \) in Eq. (92) still contains a small linear light quark mass term, \( \overline{m}(\overline{m})\alpha_s/27 \). This term arises because the heavy quark 1S mass receives, through the kinetic energy term \( -\nabla^2/M_Q^{\text{pole}} \) in the Schrödinger equation (1), an additional dependence on the pole mass. This does not affect the cancellation of linear light quark mass terms in the total static energy. The associated ambiguity exists, regardless of which of the currently known short-distance mass definitions is employed in an extraction of the bottom quark mass parameter from non-relativistic bottom–antibottom observables. However, the ambiguity is suppressed by \( \Delta^{\text{LO}} = C_2^2\alpha_s^2/8 = 0.02 \) with respect to the ambiguity of the pole mass definition, i.e. it is smaller than the order \( \Lambda_{\text{QCD}}^2/M_Q \) ambiguity for the bottom quark case. It can therefore be ignored for all practical purposes.

For simplicity we have displayed Eq. (82) for the strong coupling at the scale \( \mu = M_Q^{\text{IS}} \). Equation (82) can be generalized to arbitrary scales with the relation \( \tilde{a}_s = \alpha_s^{(n)}(M_Q^{\text{IS}}), a_s = \alpha_s^{(n)}(\mu) \):
\[ \tilde{a}_s = a_s \left\{ 1 - \epsilon \left( \frac{a_s}{2\pi} \right) \beta_0 \ln \left( \frac{M_Q^{\text{IS}}}{\mu} \right) + \epsilon^2 \left( \frac{a_s}{2\pi} \right)^2 \left[ \beta_0^2 \ln^2 \left( \frac{M_Q^{\text{IS}}}{\mu} \right) - \frac{1}{2} \beta_1 \ln \left( \frac{M_Q^{\text{IS}}}{\mu} \right) \right] \right\}. \]  

28
We note that, when we examine the scale dependence of the light quark mass corrections in the following subsection, we leave the scales of the quark masses unchanged. We also note that from now on we will designate to the terms of order $\epsilon^n$ in Eq. (82) by the expression “order $\alpha^n_s$”. This accounts for the fact that a determination of the heavy quark 1S mass at NNLO in the non-relativistic expansion corresponds to an order $\alpha^3_s$ determination of the heavy quark MS mass, as far as the proper cancellation of the linear infrared-sensitive contributions is concerned.

5.2 Brief Examination

It is instructive to examine the size of the light quark mass corrections in Eq. (82) for the case of the bottom quark ($n_l = 4$) taking into account the mass of the charm quark and treating the other light quarks as massless. For $M_b^{1S} = 4.7$ GeV, $\bar{m}(\bar{m}) = 1.5$ GeV and $\alpha_s^{(4)}(\mu = 4.7$ GeV$) = 0.216$ we obtain

$$M_b(M_b) = 4.7 - \epsilon \left[ 0.382 \right] - \epsilon^2 \left[ 0.098 + 0.0072_m \right] - \epsilon^3 \left[ 0.030 + 0.0049_m \right].$$

The corrections coming from the finite charm quark mass are indicated by the subscript “m”. The shift in $M_b(M_b)$ caused by the charm mass corrections is $-7.2 \text{ MeV}$ at order $\alpha^2_s (\epsilon^2)$ and $-4.9 \text{ MeV}$ at order $\alpha^3_s (\epsilon^3)$. If we neglect the NNLO double-insertion corrections in $\Delta_{\text{NNLO massive}}$ in Eq. (85), we obtain $-6.1 \text{ MeV}$ at order $\alpha^3_s$. It is quite instructive to confront the perturbative series of the bottom pole–MS and the bottom 1S–pole mass relations in Eqs. (34) and (53) with the result for the MS–1S mass relation in Eq. (99). For $M_b^{\text{pole}} = 4.9$ GeV and $\bar{M}_b(M_b) = 4.2$ GeV and the same values for $\alpha_s$, $\mu$ and $\bar{m}(\bar{m})$ as for Eq. (99), we obtain:

$$M_b^{\text{pole}} = 4.2 + \epsilon \left[ 0.385 \right] + \epsilon^2 \left[ 0.197 + 0.0117_m \right] + \epsilon^3 \left[ 0.142 + 0.0176_m \right],$$

$$M_b^{1S} = 4.9 - \epsilon \left[ 0.051 \right] - \epsilon^2 \left[ 0.074 + 0.0045_m \right] - \epsilon^3 \left[ 0.099 + 0.0121_m \right].$$
Table 5: The scale dependence of the “massless” (no subscript), “massive” (subscript “m”) and the large-$\beta_0$ (subscript “$b_0$”) corrections in the bottom $\overline{\text{MS}}$–1S mass relation for $m(\overline{m}) = 1.5$ GeV, $M^\text{1S}_b = 4.7$ GeV and $\alpha_s^{(5)}(M_Z) = 0.118$. The superscript “(i)” corresponds to corrections at order $\alpha_s^{(i)}$ (or $\epsilon^i$ in the epsilon expansion).

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Clearly, the bottom $\overline{\text{MS}}$–1S mass relation has a much better convergence for the corrections for massless light quarks as well as for the charm mass corrections. As expected, we find that the cancellation of the linear charm mass term is more efficient at order $\alpha_s^3$ ($\epsilon^3$) than at order $\alpha_s^2$ ($\epsilon^2$). In Fig. 3a the scale dependence of the charm mass corrections $M^\text{1S}_b(\Delta_m^{(2)} + \Delta_m^{(3)})$ is displayed for $M^\text{1S}_b = 4.7$ GeV and $\alpha_s^{(5)}(M_Z) = 0.118$ for $m(\overline{m}) = 0.1$ GeV (dotted line), 1.0 GeV (dash-dotted line), 1.5 GeV (dashed line) and 2.0 GeV (solid line). For the strong coupling we have employed four-loop running and three-loop matching conditions at the five-four quark flavour threshold. In Table 5 the scale dependence of the “massless” and “massive” corrections in Eq. (82) are shown for $m(\overline{m}) = 1.5$ GeV, $M^\text{1S}_b = 4.7$ GeV and $\alpha_s^{(5)}(M_Z) = 0.118$, separately for each order. We see that the convergence of the charm mass corrections is best for $\mu \approx m(\overline{m})$, whereas for the massless corrections this happens for $\mu \approx 2.5$ GeV. This reflects that the characteristic scales for the two types of corrections are slightly different. This is not unexpected as the relevant dynamical scales for the charm mass corrections are the charm mass and the inverse Bohr radius $M_b\alpha_s$; the massless corrections, on the other hand, involve $M_b$ and $M_b\alpha_s$ as relevant dynamical scales. The convergence of the charm mass corrections shown in Table 5 clearly shows that they are well under control. For our final determination of the bottom quark $\overline{\text{MS}}$ mass in Sec. 7, we will use renormalization scales between 1.5 and 7 GeV. For the determination of the central value of the bottom $\overline{\text{MS}}$ mass we will use $\mu = M^\text{1S}_b$.

In Fig. 3b, finally, the size of the charm mass correction $M^\text{1S}_b(\Delta_m^{(2)} + \Delta_m^{(3)})$ is plotted over $m(\overline{m})$ for $M^\text{1S}_b = 4.7$ GeV, $\alpha_s^{(5)}(M_Z) = 0.118$ and $\mu = 1.5$ GeV (dotted line), 3 GeV (dashed line) and 5 GeV
MS–1S mass relation in Eq. (82) contains \( M_{b}(\overline{\text{MS}}) \). Figures 3a and b show that for \( m(\overline{m}) = 0.1 \) GeV the corrections amount to much less than 1 MeV. Thus, the effects of the masses from light quarks other than the charm can be safely neglected.

5.3 Estimate of the Order \( \alpha_s^4 \) Charm Mass Effects

The results shown in the 9th and the 10th row of Table 5 reveal a quite interesting property of the ratio between the full corrections and the massless ones at order \( \alpha_s^2 \) and \( \alpha_s^3 \). For \( \mu \) around 4 to 5 GeV the ratios at order \( \alpha_s^2 \) and \( \alpha_s^3 \) are approximately equal to \( (\beta_0^{(n=3)}/\beta_0^{(n=4)}) = 1.08 \) and \( (\beta_0^{(n=3)}/\beta_0^{(n=4)})^2 = 1.17 \), respectively. We already mentioned that the inclusion of the charm mass leads to an effective decoupling of the charm quark corrections at large orders. Thus, because the order \( \alpha_s^{n+1} \) term in the \( \overline{\text{MS}}–1\S \) mass relation in Eq. (82) contains \( \beta_0^n \), the value \( (\beta_0^{(n=3)}/\beta_0^{(n=4)})^n \) for the ratio might not be unexpected as the asymptotic behaviour for large orders of perturbation theory. However, we emphasize that if ones employs \( \alpha_s^{(n=4)} \) rather than \( \alpha_s^{(n=3)} \), as we do in this work, the decoupling is not explicit. (See the results for the light quark mass corrections for the static potential discussed in Sec. 2.) In addition, because the series in the bottom \( \overline{\text{MS}}–1\S \) mass relation in Eq. (82) involves the cancellation of the leading infrared-sensitive contributions, also subleading contributions, which involve for example \( \beta_1 \), lower powers of \( \beta_0 \) or higher order contributions in the non-relativistic expansion, will contribute to the dominant asymptotic behaviour of the perturbative coefficients in Eq. (82). Thus the observation above is certainly a coincidence, particularly the one at order \( \alpha_s^2 \). Nevertheless, the ratio \( (\beta_0^{(n=3)}/\beta_0^{(n=4)})^n \) might be used as a rough estimate for the large order behaviour of the ratio of full to massless corrections in the \( \overline{\text{MS}}–1\S \) mass relation. It should therefore be possible to estimate the size of the order \( \alpha_s^4 \) charm mass corrections \( \Delta_m^{(4)} \) from the order \( \alpha_s^4 \) corrections for massless light quarks, \( \Delta^{(4)} \). At the present stage the full result for \( \Delta^{(4)} \) is not yet known. However, it can be rather easily calculated in the large-\( \beta_0 \) approximation because for the N\(^3\)LO corrections to the pole–1S mass relation this only amounts to the insertion of one-loop massless quark vacuum polarizations into the LO static potential. The order \( \alpha_s^4 \) large-\( \beta_0 \) corrections to the pole–\( \overline{\text{MS}} \) mass relation are already known from Ref. [41], whereas the N\(^3\)LO corrections to the pole–1S mass relation in the large-\( \beta_0 \) approximation are calculated in App. B. The formula for \( \Delta^{(4)} \) in the large-\( \beta_0 \) approximation is derived in App. C and reads (\( \tilde{\alpha}_s = \alpha_s^{(4)}(M_t^{\text{LO}}) \))

\[
\Delta^{(4)}_{\beta_0} = \frac{C_F}{8} \frac{\tilde{\alpha}_s^2}{\pi} \left[ \frac{1}{2} \tilde{L}^3 + \frac{15}{8} \tilde{L}^2 + \left( \frac{\pi^2}{12} + \frac{\zeta_3}{12} + \frac{25}{12} \right) \tilde{L} 
+ \frac{\pi^4}{1440} + \frac{19 \pi^2}{144} + \frac{3}{2} \tilde{\zeta}_5 - \left( \frac{\pi^2}{8} - \frac{11}{6} \right) \zeta_3 + \frac{517}{684} \right]
- \left( \frac{\tilde{\alpha}_s}{\pi} \right)^4 \frac{\beta_0^3}{6} \left( \frac{71 \pi^4}{7680} + \frac{317}{768} \zeta_3 + \frac{89 \pi^2}{1152} + \frac{42979}{331776} \right),
\]

(102)

where \( \tilde{L} = \ln(1/C_F \tilde{\alpha}_s) \). Equation (102) can be generalized to arbitrary renormalization scales in the strong coupling using the one-loop running of the strong coupling, in analogy to Eq. (98), which only involves corrections proportional to \( \beta_0 \). We have displayed the scale dependence of \( M_t^{\text{LO}} \Delta^{(i)}_{\beta_0} \) (\( i = 1, 2, 3, 4 \)) for \( m(\overline{m}) = 1.5 \) GeV, \( M_t^{\text{LO}} = 4.7 \) GeV and \( \alpha_s^{(5)}(M_Z) = 0.118 \) in the 11th to the 14th rows of Table 5. The values for very small choices of \( \mu \) are meaningless. As indicated in the discussion about the ratio \( (\beta_0^{(3)}/\beta_0^{(4)})^n \) at the beginning of this subsection, we see that the large-\( \beta_0 \)
approximation does certainly not provide a very good estimate of the true corrections. At order $\alpha_s^2$ and $\alpha_s^3$ the large-$\beta_0$ result overestimates the true correction. For $\mu \gtrsim 3$ GeV the difference is between 50 and 100%. This demonstrates that the large-$\beta_0$ approximation does in general not give more than an order of magnitude estimate if it is applied to a perturbative expansion that does not contain a linear sensitivity to small momenta, as is the case in the $\overline{\text{MS}}$–1S mass relation. (In the pole-$\overline{\text{MS}}$ mass relation, which contains a linear sensitivity to small momenta, the large-$\beta_0$ approximation is considerably better, see e.g. Ref. [41].) On the other hand, the large-$\beta_0$ approximation seems to indicate quite a good convergence for larger values of $\mu$. Although we cannot prove that this property allows for any conclusion about the size of the true expression for $M_{1S}^{\text{MS}}$–$\Delta^{(4)}$, we believe that this is likely to be the case. If the relative size of the large-$\beta_0$ corrections roughly reflects the relative size of the true corrections, one can expect that $M_{1S}^{\text{MS}}$–$\Delta^{(4)}$ amounts to around $-10$ to $-15$ MeV for $\mu$ around 5 GeV. Using the value $(\beta_0^{(3)}/\beta_0^{(4)})^3 = 1.26$ as an estimate for the ratio $(\Delta^{(4)} + \Delta_m^{(4)})/\Delta^{(4)}$, this results in $\Delta_m^{(4)} = -3$ to $-4$ MeV for $\mu$ around 5 GeV. This estimate seems to be consistent with the sum $M_{1S}^{\text{MS}}(\Delta_m^{(2)} + \Delta_m^{(3)})$ at the scale $\mu = 1.5$ GeV, where we find the best convergence of the charm mass corrections.

To conclude the somewhat speculative discussion of this subsection, we note that the main outcome is that the large-$\beta_0$ approximation does not provide a particularly good estimate of higher order corrections in the $\overline{\text{MS}}$–1S mass relation. This is because subleading infrared-sensitive contributions would have to be taken into account to determine the dominant asymptotic behaviour of the perturbative relation of short-distance masses. As far as our estimate for the order $\alpha_s^4$ charm mass corrections in the bottom $\overline{\text{MS}}$–1S mass relation is concerned, we believe that it is more likely to be correct than the estimate for the order $\alpha_s^4$ massless corrections, as the light quark mass corrections at order $\alpha_s^4$ do not yet contain any ultrasoft contributions.

6 Light Quark Mass Effects in the $\Upsilon$ Sum Rules

In this section we determine the corrections coming from the finite charm quark mass to the large-$n$ moments of the bottom–antibottom quark cross section in $e^+e^-$ annihilation at NNLO in the non-relativistic expansion. In Sec. 6.1 we briefly review the basic concepts involved in the $\Upsilon$ sum rules. More details can be found in Ref. [7]. In Sec. 6.2 we outline our method to calculate the moments, and in Sec. 6.3 we present the calculations of the charm mass corrections. Results for the calculations for massless light quarks are not given here; they have been given in Ref. [7]. In Sec. 6.4 the results for the charm mass corrections are examined.

6.1 Basic Issues

The sum rules for the $\Upsilon$ mesons start from the correlator of two electromagnetic currents of bottom quarks at momentum transfer $q$,

\[
\Pi_{\mu\nu}(q) = -i \int dx e^{ix\cdot q} \langle 0 | T j^b_\mu(x) j^b_\nu(0) | 0 \rangle
\]

---

8 We are aware of the fact that $\Delta^{(3)}$ contains ultrasoft “Lamb-shift”-type corrections that involve $M_b\alpha_s^2$ as the relevant dynamical scale and might lead to considerable additional contributions. Calculations of the latter have been carried out in Refs. [42, 43]. However, no concrete statement can be made before all corrections in $\Delta^{(4)}$ are determined.
\[ \equiv \text{Im} \left[ -i \langle 0 | T \bar{J}_{\mu}^b(q) J^b_{\mu}(-q) | 0 \rangle \right], \quad (103) \]

where
\[ J_{\mu}^b(x) = \bar{b}(x) \gamma_{\mu} b(x), \quad (104) \]

and the symbol \( b \) denotes the bottom quark Dirac field. The \( n \)-th moment \( P_n \) of the vacuum polarization function is defined as
\[ P_n \equiv \frac{4 \pi^2 Q_b^2}{n! q^2} \left( \frac{d}{dq^2} \right)^n \Pi^\mu_\mu(q^2) \bigg|_{q^2=0}, \quad (105) \]

where \( Q_b = -1/3 \) is the electric charge of the bottom quark. Due to causality the \( n \)-th moment \( P_n \) can also be written as a dispersion integral
\[ P_n = \int_{\sqrt{s_{\text{min}}}}^{\infty} \frac{ds}{s^{n+1}} R(s), \quad (106) \]

where
\[ R(s) = \frac{\sigma(e^+e^- \rightarrow \gamma^* \rightarrow \bar{b}b+X)}{\sigma_{pt}} = \frac{4 \pi Q_b^2}{s} \text{Im} \Pi^\mu_\mu(s) \quad (107) \]

is the total photon-mediated cross section of bottom quark–antiquark production in \( e^+e^- \) annihilation normalized to the Born cross section for massless leptons, \( \sigma_{pt} \equiv 4 \pi \alpha^2 / 3s \), and \( s \) is the square of the centre-of-mass energy. The lower limit of the integration in Eq. (106) is set by the mass of the lowest-lying resonance. Assuming global duality the moments \( P_n \) can be either calculated from experimental data on \( R \) or theoretically using perturbative QCD.

The experimental moments \( P_n^{\text{ex}} \) are determined by using latest data on the \( \Upsilon \) meson masses, \( M_{kS} \), and electronic decay widths, \( \Gamma_{kS} \), for \( k = 1, \ldots, 6 \). The formula for the experimental moments used in this work reads
\[ P_n^{\text{ex}} = \frac{9 \pi}{\tilde{\alpha}_{\text{em}}^2} \sum_{k=1}^{6} \frac{\Gamma_{kS}}{M_{kS}^{2n+1}} + \int_{(\sqrt{s})_{\text{BB}}}^{\infty} \frac{ds}{s^{n+1}} r_{\text{cont}}(s), \quad (108) \]

and is based on the narrow width approximation for the known \( \Upsilon \) resonances; \( \tilde{\alpha}_{\text{em}} \) is the electromagnetic coupling at the scale 10 GeV. Because the difference in the electromagnetic coupling for the different \( \Upsilon \) masses is negligible, we chose 10 GeV as the scale of the electromagnetic coupling for all resonances. The continuum cross section above the \( BB \) threshold is approximated by the constant \( r_c = 1/3 \), which is equal to the Born cross section for \( s \rightarrow \infty \), assuming a 50% uncertainty,
\[ r_{\text{cont}}(s) = r_c(1 \pm 0.5). \quad (109) \]

For \( n \geq 4 \) the continuum contribution is already suppressed sufficiently so that a more detailed description is not needed. For a compilation of all experimental numbers used in this work, see Table 6.

A reliable computation of the theoretical moments \( P_n^{\text{th}} \) based on perturbative QCD is only possible if the effective energy range contributing to the integration in Eq. (106) is sufficiently larger than \( \Lambda_{\text{QCD}} \sim \mathcal{O}(200–300 \text{ MeV}) \) [45]. For large values of \( n \) it can be shown that the size of this energy range is of order \( M_b/n \). Qualitatively this dependence on the moment parameter \( n \) can be seen from
<table>
<thead>
<tr>
<th>nS</th>
<th>$M_{nS}/[\text{GeV}]$</th>
<th>$\Gamma_{nS}/[\text{keV}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1S</td>
<td>9.460</td>
<td>1.32 ± 0.04 ± 0.03</td>
</tr>
<tr>
<td>2S</td>
<td>10.023</td>
<td>0.52 ± 0.03 ± 0.01</td>
</tr>
<tr>
<td>3S</td>
<td>10.355</td>
<td>0.48 ± 0.03 ± 0.03</td>
</tr>
<tr>
<td>4S</td>
<td>10.58</td>
<td>0.25 ± 0.03 ± 0.01</td>
</tr>
<tr>
<td>5S</td>
<td>10.87</td>
<td>0.31 ± 0.05 ± 0.07</td>
</tr>
<tr>
<td>6S</td>
<td>11.02</td>
<td>0.13 ± 0.03 ± 0.03</td>
</tr>
</tbody>
</table>

Table 6: The experimental numbers for the $\Upsilon$ masses and electronic decay widths used for the calculation of the experimental moments $P_{n}^{\text{ex}}$. For the widths, the first error is statistical and the second one systematic. The errors for the partial widths of $\Upsilon(1S)$ and $\Upsilon(2S)$ are taken from Ref. [44]. All the other errors are estimated from the numbers presented in Ref. [28]. For the electromagnetic coupling at 10 GeV and the $B\bar{B}$ threshold we use $\tilde{\alpha}_{\text{em}}^{-1} = \alpha_{\text{em}}^{-1}(10 \text{GeV}) = 131.8(1 \pm 0.005)$ and $(\sqrt{s})_{BB} = 2 \times 5.279$ GeV. The small errors in the $\Upsilon$ masses and the $B\bar{B}$ threshold $(\sqrt{s})_{BB}$ are neglected.

Eq. (106): large values of $n$ enhance the low energy contributions and suppress the high energy ones. This implies that $n$ should be chosen sufficiently smaller than 15–20. This is consistent with estimates of non-perturbative effects in the large-$n$ moments using the gluon condensate [4, 46]:

$$P_{n}^{\text{non-pert}} \approx P_{n}^{\text{th}} \left[ 1 - \left( \frac{n^3 \pi}{72 M_b^4} \alpha_s \frac{\sqrt{n}}{4 C_F} \right) \exp \left( -0.4 C_F \alpha_s \sqrt{n} \right) \right],$$

(110)

where the $P_{n}^{\text{th}}$ represent the theoretical moments obtained with pure perturbation theory. The RHS of Eq. (110) amounts to less than a per cent of the theoretical moments for $n < 20$. However, this result needs some careful interpretation because the estimate of non-perturbative effects based on an expansion in gluonic and light quark condensates is only reliable if $M_b v^2 \gg \Lambda_{\text{QCD}}$. In addition, the values of the dimension-6 (and higher) condensates as well as all perturbative Wilson coefficients for the condensates are unknown, which introduces additional systematic uncertainties. In order to suppress these sources of uncertainties, $n$ should be chosen as small as possible. However, it is also desirable to choose $n$ as large as possible in order to suppress the contribution from the $b\bar{b}$ continuum to $R(s)$ above the $BB$ threshold, which is rather poorly known experimentally. In other words, one has to choose $n$ large enough for the bottom–antibottom quark dynamics encoded in the moments $P_n$ to be non-relativistic. Because the size of the energy range contributing to the $n$-th moment is of order $M_b/n$, the mean centre-of-mass velocity of the bottom quarks in the $n$-th moment is $v \sim 1/\sqrt{n}$. This counting rule allows for a quantitative formulation of the two requirements for the choice of $n$: theoretical reliability demands $M_b v^2 \gg \Lambda_{\text{QCD}}$, and dominance of the non-relativistic dynamics demands $v \ll 1$. If both requirements are met, the bottom–antibottom quark dynamics encoded in the moments is perturbative, i.e. the hierarchy $M_b \gg M_b v \gg M_b v^2 \gg \Lambda_{\text{QCD}}$ is valid. Only if this condition is satisfied, the non-relativistic power counting described after Eq. (1) and used throughout this work is truly justified. Only in this case can the non-relativistic bottom–antibottom quark pair be considered as a Coulombic system for which the perturbative treatment carried out in this work is
feasible and for which the power counting
\[ v \sim \alpha_s \sim \frac{1}{\sqrt{n}}, \]  
used for the calculation of the moments, can be applied. In our analysis we choose
\[ 4 \leq n \leq 10 \]  
as the allowed range for the moments \( P_n \). The upper bound was chosen to avoid the problem of unknown systematic non-perturbative uncertainties as much as possible. The gluon condensate contributions mentioned above amounts to less than a per mille in the moments for \( n \leq 10 \). This is an order of magnitude less than the charm mass corrections. Therefore, non-perturbative effects are not taken into account in this work. The lower bound, on the other hand, is a compromise born out of the requirement of the non-relativistic dominance and of the fact that we would like to have a reasonable number of moments that can be used for fitting. We also note that our estimate of the size of non-perturbative effects is based on the common faith that the expansion in gluon condensates really describes the dominant source of non-perturbative contributions. This is not necessarily the case, as has been pointed out for instance in Refs. [47]. As we will discuss in Sec. 6.4, the perturbative behaviour of the moments does not seem to comply at all the estimate of the smallness of non-perturbative effects based on the gluon condensate (presuming that perturbative convergence has anything to do with the size non-perturbative effects). We believe that it is probably the weakest point of the sum rule method.

6.2 Method for the Calculation of the Moments

In this subsection we briefly review the method used in Ref. [7] for the calculation of the NNLO moments for massless light quarks assuming the pole definition for the bottom mass. This sets the stage for the determination of the charm mass corrections carried out in Sec. 6.3.

At NNLO in the non-relativistic expansion, we need to calculate corrections up to order \( \alpha_s^2, \alpha_s/\sqrt{n} \) and \( 1/n \) to the moments \( P_n \) with respect to the non-relativistic (LO) limit. According to the power counting (111) we need to keep corrections of order \( \alpha_s^2, \alpha_s v \) and \( v^k n^l \) with \( k - 2l = 2 \) in the non-relativistic expansion of Eq. (106),

\[ P_n^{\text{th}} = \frac{1}{4^n (M_b^{\text{pole}})^{2n}} \int_{E_{\text{bind}}}^{\infty} \frac{dE}{M_b^{\text{pole}}} \exp \left( -\frac{E}{M_b^{\text{pole}}} n \right) \left( 1 - \frac{E}{2 M_b^{\text{pole}}} + \frac{E^2}{4 (M_b^{\text{pole}})^2 n} \right) R_{\text{NNLO}}^{\text{thr}}(E), \]  
where \( E = \sqrt{s} - 2 M_b^{\text{pole}} \) and \( E_{\text{bind}} \) is the perturbative binding energy of the lowest-lying resonance, i.e. \( E_{\text{bind}} = 2(M_b^{1S} - M_b^{\text{pole}}) \). The exponential \( \exp(-E/M_b^{\text{pole}} n) \) is the LO term in the non-relativistic expansion of \( ds/s^{n+1} \) and cannot be expanded because \( E/M_b^{\text{pole}} n \) is of order 1 according to the power counting of Eq. (111). We note that the non-relativistic expansion of \( ds/s^{n+1} \) does not contain any NLO corrections, as these would be non-analytic functions of the energy \( E \). Thus, because the light quark mass corrections start at NLO, we only need to consider the LO term in the non-relativistic expansion of \( ds/s^{n+1} \) in the determination of the light quark mass corrections up to NNLO. The term \( R_{\text{NNLO}}^{\text{thr}} \) is the bottom–antibottom quark cross section expanded at NNLO in the non-relativistic
expansion. It is obtained by expanding the relativistic electromagnetic bottom quark currents in Eq. (107) in terms of effective non-relativistic $^3S_1$ currents up to dimension 5 ($i = 1, 2, 3$):

\[ \tilde{j}_i^b(q) = c_1 \left( \bar{\psi}^i \sigma_i \bar{\chi} \right)(q) - \frac{c_2}{6M_b^2} \left( \bar{\psi}^i \sigma_i \left(-\frac{i}{2} \overrightarrow{D} \right)^2 \bar{\chi} \right)(q) + \ldots, \]  

where $s = q^2$. The non-relativistic currents are defined in the NRQCD factorization scheme proposed by Lepage et al., which separates contributions coming from momenta of order $M_b$ from non-relativistic momenta of order $M_b v$ and $M_b v^2$. The constants $c_1$ and $c_2$ are short-distance Wilson coefficients that contain the contributions from momenta of order $M_b$. At the Born level, $c_1 = c_2 = 1$. At NNLO we need $c_1$ at order $\alpha_s^2$; for $c_2$ we do not need to calculate any corrections as the contributions of dimension-5 currents are already suppressed by two powers of $v$. From Eqs. (114) and (115) one obtains

\[ R_{\text{NNLO}}(E) = \frac{\pi Q_b^2}{(M_b^{\text{pole}})^2} C_1(\mu_{\text{hard}}, \mu_{\text{fac}}) \text{Im} \left[ A_1(E, \mu_{\text{soft}}, \mu_{\text{fac}}) \right] \]

\[ - \frac{4\pi Q_b^2}{3(M_b^{\text{pole}})^2} \text{Im} \left[ A_2(E, \mu_{\text{soft}}) \right] + \ldots, \]  

where $C_1 = c_1^2$ and

\[ A_1 \equiv i \langle 0 | (\bar{\psi}^i \sigma_i \bar{\chi}) (\bar{\chi}^\dagger \sigma \bar{\psi}) | 0 \rangle, \]  

\[ A_2 \equiv \frac{1}{2} i \langle 0 | (\bar{\psi}^i \sigma_i \bar{\chi}) (\bar{\chi}^\dagger \sigma \left(-\frac{i}{2} \overrightarrow{D} \right)^2 \bar{\psi}) + \text{h.c.} | 0 \rangle. \]  

The constant $Q_b = -1/3$ is the electric charge of the bottom quark. Using the NRQCD equation of motion for the bottom and antibottom quark fields, one can relate $A_2$ to $A_1$, $A_2 = M_b^{\text{pole}} E A_1$. In Eq. (116) we have indicated the dependence of the non-relativistic cross section on the renormalization scales used in Refs. [7, 9]. The scale $\mu_{\text{soft}}$ is the renormalization scale of the strong coupling governing the bottom–antibottom quark potential in Eq. (1) and $\mu_{\text{hard}}$ the renormalizations scale of the strong coupling in the short-distance coefficient $C_1$. The scale $\mu_{\text{fac}}$ is a factorization scale that separates non-relativistic from hard momenta in the NRQCD factorization scheme. The scales $\mu_{\text{hard}}$, $\mu_{\text{fac}}$ are irrelevant to the charm quark mass corrections determined in this work, since they contain no hard corrections up to NNLO. The dimension-6 current correlator $A_1$ is obtained at NNLO from the configuration space Green function of Eq. (1) for both spatial arguments evaluated at zero distance:

\[ A_1 = 6 N_c G(0, 0, E). \]  

(See Ref. [39] for details on the derivation of Eq. (119).) The short-distance coefficient $C_1$ is obtained by matching the NNLO cross section in Eq. (116) to the same cross section in full QCD in the (formal) limit $\alpha_s \ll v \ll 1$ at the two-loop level and including terms in the velocity expansion up to NNLO. This method of determining the short-distance coefficient $C_1$ at the level of the cross section (rather than the amplitude) is called “direct matching” [50]. The calculation of the NNLO zero-distance Green function
of the Schrödinger equation (1) proceeds in analogy to the determination of the NNLO corrections to the 1S mass carried out in Sec. 4 via Rayleigh–Schrödinger time-independent perturbation theory. Parametrizing the zero-distance Green function as

$$\ G(0,0,E) \ = \ G_c(0,0,E) + G_{\text{NLO}}(0,0,E) + G_{\text{NNLO}}(0,0,E), \quad (120)$$

where $G_c$ is the LO non-relativistic Coulomb Green function, the formal expressions for $G_{\text{NLO}}$ and $G_{\text{NNLO}}$ at zero distances read ($r \equiv |r|$, $r' \equiv |r'|$):

$$G_{\text{NLO}}(0,0,E) = - \int d^3r \ G_c(0,r,E) V_{\text{c,massless}}^{\text{NLO}}(r) G_c(r,0,E), \quad (121)$$

$$G_{\text{NNLO}}(0,0,E) = - \int d^3r \ G_c(0,r,E) \left( V_{\text{c,massless}}^{\text{NLO}}(r) + V_{\text{BF}}(r) + V_{\text{NA}}(r) + \delta H_{\text{kin}} \right) G_c(r,0,E)$$

$$+ \int d^3r \int d^3r' \ G_c(0,r,E) V_{\text{c,massless}}^{\text{NLO}}(r) G_{\text{c}}(r,0,E) V_{\text{c,massless}}^{\text{NLO}}(r') G_c(r',0,E) \quad (122)$$

in configuration space representation, where $\delta H_{\text{kin}} = -\nabla^4/4M_{b}$.

The expressions for the Coulomb Green function in Eqs. (123) and (124) have been derived in Refs. [51]. For the NNLO contributions arising from second order Rayleigh–Schrödinger perturbation theory we only need the S-wave component of the Coulomb Green function, $G_c^S$, for the sum over intermediate states because the static potential at NLO is spin- and angle-independent. The case $r < r'$ in Eq. (123) is obtained by interchanging $r$ and $r'$.

The calculation of the moments as shown in Eq. (113) is somewhat cumbersome, because it requires the separate determination of bound state ($E < 0$) and continuum ($E > 0$) contributions. In particular, for the bound state contributions, the binding energies and the leptonic decay rates (which are proportional to the modulus squared of the configuration space wave functions at the origin) of all resonances would need to be determined individually. A more economic way to calculate the moments can be achieved by deforming the path of integration in Eq. (113) into the negative complex plane, as
Figure 4: Path of integration to calculate expression (127) for the theoretical moments. The dashed line closes the contour at infinity and does not contribute to the integration. The free constant $\gamma$ is chosen large enough to be safely away from the bound state poles, which are indicated by the grey dots on the negative energy axis. The thick grey line on the positive energy axis represents the continuum.

shown in Fig. 4. Because the path that closes the contour at infinity does not contribute, the result of the integration in Eq. (113) can be written as

$$ P_n^{\text{th}} = \frac{-2iQ_b^2\pi}{(4M_b^2)^{n+1}} \int_{-\gamma-i\infty}^{\gamma+i\infty} \frac{dE}{M_b} \exp\left( -\frac{E}{M_b} \right) \left( 1 - \frac{E}{2M_b} + \frac{E^2}{4M_b^2} \right)^n \left[ C_1A_1(E) - \frac{4}{3M_b^2}A_2(E) \right] $$

$$ = \frac{4Q_b^2\pi^2}{(4M_b^2)^{n+1}} \frac{1}{2\pi i} \int_{-\gamma-i\infty}^{\gamma+i\infty} \frac{d\tilde{E}}{M_b} \exp\left( \frac{\tilde{E}}{M_b} n \right) \left( 1 + \frac{\tilde{E}}{2M_b} + \frac{\tilde{E}^2}{4M_b^2} n \right)^n \left[ C_1A_1(-\tilde{E}) - \frac{4}{3M_b^2}A_2(-\tilde{E}) \right], $$

(127)

where the free constant $\gamma$ is chosen much larger than the ground state binding energy $E_{\text{bind}}$. In the second line of Eq. (127) the change of variable $E \rightarrow -\tilde{E}$ has been performed. We note that, in contrast to Eq. (113), we also need the real part of the correlators $A_1$ and $A_2$ in Eq. (127). The expression in Eq. (127) has three advantages: (i) the bound state and continuum contributions are obtained at the same time, (ii) the correlators, i.e. the Green functions shown in Eq. (120), can be naively expanded in $\alpha_s$ before the integration, and (iii) we can use a vast number of tables for the calculations, because the complex energy integration is nothing else than an inverse Laplace transform. This elegant way to determine the moments has been used first in Ref. [4].

The final result for the NNLO theoretical moments for massless light quarks can be cast into the form

$$ P_n^{\text{th}} = \frac{3N_cQ_b^2\sqrt{\pi}}{4^{n+1}(M_b^{\text{pole}})^{2n}n^{3/2}} \left\{ C_1\left( \frac{\mu_{\text{hard}}}{M_b^{\text{pole}}}, \frac{\mu_{\text{fac}}}{M_b^{\text{pole}}}, \alpha_s(\mu_{\text{hard}}) \right) g_{n,1}\left( \frac{\mu_{\text{soft}}}{M_b^{\text{pole}}}, \frac{\mu_{\text{fac}}}{M_b^{\text{pole}}}, \alpha_s(\mu_{\text{soft}}) \right) \right. $$

$$ + \left. g_{n,2}\left( \alpha_s(\mu_{\text{soft}}) \right) \right\}, $$

(128)
\[ \varrho_{n,1} = \frac{8 \pi^{3/2} n^{3/2}}{(M_{\text{pole}}^b)^2} \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \frac{d\tilde{E}}{M_{\text{pole}}^b} \exp \left( \frac{\tilde{E}}{M_{\text{pole}}^b} \right) \left( 1 + \frac{\tilde{E}}{2M_{\text{pole}}^b} + \frac{\tilde{E}^2}{4(M_{\text{pole}}^b)^2} \right) n G(0,0,-\tilde{E}), \]

(129)

\[ \varrho_{n,2} = \frac{8 \pi^{3/2} n^{3/2}}{(M_{\text{pole}}^b)^2} \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} \frac{d\tilde{E}}{M_{\text{pole}}^b} \exp \left( \frac{\tilde{E}}{M_{\text{pole}}^b} \right) \left( 4 \frac{\tilde{E}}{3 M_{\text{pole}}^b} \right) G_c(0,0,-\tilde{E}). \]

(130)

The explicit results for \( \varrho_{n,1} \) and \( \varrho_{n,2} \) can be found in Ref. [7]. We note that \( \varrho_{n,1} \) and \( \varrho_{n,2} \) are dimensionless and that \( \varrho_{n,1} \) depends only logarithmically on the bottom pole mass at NLO and NNLO through the dependence of the strong coupling on the inverse Bohr radius. We also note that only \( \varrho_{n,1} \) receives light quark mass corrections, since \( \varrho_{n,2} \) contains only NNLO contributions.

### 6.3 Light Quark Mass Corrections to the Moments

The light quark mass corrections to the moments are determined following the lines of the calculation for massless light quarks described in the previous subsection. The insertions of the NLO and NNLO static potentials that are needed are in complete analogy to the calculation of the heavy quark 1S mass presented in Sec. 4.

**Light Quark Mass Corrections at NLO**

The NLO light quark mass corrections to the zero-distance Green function read

\[ G_{m,\text{NLO}}(0,0,E) = - \int d^3r G_c(0,r,E) \delta V_{c,m,\text{NLO}}(r) G_c(r,0,E), \]

where the formulae for \( \delta V_{c,m,\text{NLO}} \) and \( G_c \) are given in Eqs. (18) and (124), respectively; \( \delta V_{c,m,\text{NLO}}(r) \) contains a contribution from the massive light quark vacuum polarization function, called “massive” corrections in the following, and a contribution from the subtraction of the massive light quark vacuum polarization function in the limit \( m \to 0 \), called “massless” correction in the following. This subtraction is a consequence of our convention that \( n_l \) quark species contribute to the evolution of the strong coupling.

For the massless corrections we can recycle the results for massless light quarks given in Ref. [7]. The massive corrections to the zero-distance Green function involve the term \( (a_s = \alpha_s(4)(\mu_{\text{soft}})) \):

\[ - \int d^3r G_c(0,r,E) \left[ \left( - \frac{C_F a_s}{\pi} \right) \int_1^\infty dx f(x) e^{-2mx} \right] G_c(r,0,E) \]

\[ = C_F a_s \frac{(M_{\text{pole}}^b)^2 k^2}{\pi} \int_1^\infty dx f(x) \int_0^\infty dt \int_0^\infty du \int_0^\infty dr e^{-2[k(1+t+u)+mx]} r \left( \frac{1+u}{t} \right)^{\lambda} \left( \frac{1+t}{u} \right)^{\lambda} \]

\[ = C_F a_s \frac{(M_{\text{pole}}^b)^2}{4\pi} \sum_{p=0}^{\infty} \int_1^\infty dx f(x) \int_0^\infty dt \int_0^\infty du \frac{\lambda^p}{p!} \ln^{p} \left( \frac{1+t}{u} \right) \left( \frac{1+u}{t} \right) \frac{\tilde{k}^2}{(1+t+u)^2(k+\tilde{a})^2}, \]

(132)
\[ \tilde{k} \equiv \frac{k}{M_b^{\text{pole}}}, \quad (133) \]

\[ \tilde{a} \equiv \frac{m x}{M_b^{\text{pole}} (1 + t + u)}, \quad (134) \]

and \( k \) and \( \lambda \) are defined in Eqs. (125) and (126), respectively. In the last line of Eq. (132) we have expanded in \( \alpha_s \) owing to the integration path in the negative complex energy plane shown in Eq. (127).

To determine the contributions of Eq. (132) to the light quark mass corrections of the moments \( \varrho_{n,1} \), we use the following inverse Laplace transform \([52]\):

\[ \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{z^{-p}}{(z + A)^2} e^{z^2 n} = n^{\frac{p}{2} - 1} g_0(p, A^2 n), \quad (135) \]

where

\[ g_0(p, X) = \frac{1 + 2 X}{\Gamma(\frac{p}{2})} - \frac{2 \sqrt{X} (1 + X)}{\Gamma(\frac{1+p}{2})} + e^X X^{1 - \frac{p}{2}} (3 - p + 2 X) \left[ \frac{\Gamma(\frac{1+p}{2}, X)}{\Gamma(\frac{1+p}{2})} - \frac{\Gamma(\frac{p}{2}, X)}{\Gamma(\frac{p}{2})} \right], \quad (136) \]

The final result for the NLO light quark mass corrections to the moments reads

\[ \delta \varrho_{n,1}^{\text{NLO}} = 4 \sqrt{\pi} \left( \frac{a_s}{3 \pi} \right) \phi \left\{ \frac{1}{2} \int_1^\infty dx f(x) e^{n x^2} \left[ 1 - \text{erf}(\sqrt{n} x) \right] + \sum_{p=1}^{\infty} \phi^p \bar{g}_0(n, p, \eta) \right\} \]

\[ + \left[ \frac{1}{2} \ln \left( \frac{\eta \sqrt{n}}{2} \right) + \frac{\gamma_\text{E}}{4} + \frac{5}{12} + \sum_{p=1}^{\infty} \phi^p \left( w_0^p \left( \frac{1}{2} \Psi \left( \frac{p}{2} \right) - \ln \left( \frac{\eta \sqrt{n}}{2} \right) - \frac{5}{6} \right) + w_1^p \right) \right], \quad (137) \]

where

\[ \phi \equiv \frac{C_F a_s \sqrt{n}}{2}, \quad (138) \]

\[ \eta \equiv \frac{m}{M_b^{\text{pole}}}, \quad (139) \]

and

\[ \bar{g}_0(n, p, \eta) = \int_0^\infty dt \int_0^\infty du \int_1^\infty dx f(x) \frac{1}{p! (1 + t + u)^2} \ln^p \left( \frac{(1 + t)(1 + u)}{t u} \right) g_0(p, X) \bigg|_{X = \frac{\eta \sqrt{n}}{2}}, \quad (140) \]

The first term in the curly brackets on the RHS of Eq. (137) comes from the massive corrections and the second from the massless ones. The constants \( w_0^p \) and \( w_1^p \) have already been calculated in Ref. [7]; their expressions can be found in App. E. The function \( \bar{g}_0 \) has been calculated numerically using standard variable transforms to treat the logarithmic singularities. We note that the numerical
Light Quark Mass Corrections at NNLO – Single Insertions

The NNLO light quark mass corrections to the zero-distance Green function read

\[
\delta G^{\text{NNLO}}_{m}(0,0,E) = - \int d^3r \ G_c(0,r,E) \delta V^{\text{NNLO}}_{c,m}(r) \ G_c(r,0,E)
\]

\[
+ \int d^3r \ \int d^3r' \ G_c(0,r,E) \delta V^{\text{NNLO}}_{c,m}(r) \ G^S_c(r',r,E) \delta V^{\text{NNLO}}_{c,m}(r') \ G_c(r',0,E)
\]

\[
+ 2 \int d^3r \ \int d^3r' \ G_c(0,r,E) \delta V^{\text{NNLO}}_{c,m}(r) \ G^S_c(r',r,E) \ V^{\text{NLO}}_{c,\text{massless}}(r') \ G_c(r',0,E).
\]

(141)

Let us first consider the contributions from the single insertion of the NNLO light quark mass corrections to the static potential at first order Rayleigh–Schrödinger perturbation theory. As for the NLO calculation, we distinguish between “massive” and “massless” corrections and only give details for the massive contributions. Apart from expression (132) there is one more term coming from the light quark mass corrections to the NNLO static potential that is relevant for the massive corrections:

\[
- \int d^3r \ G_c(0,r,E) \left[ \frac{C_F a_s}{r} \int_1^\infty dx \ f(x) \ e^{-2mr^2} \left( \ln(4x^2) - \text{Ei}(2mxr) - \text{Ei}(-2mxr) \right) \right] G_c(r,0,E)
\]

\[
= - C_F a_s \left( \frac{M^\text{pole}_b}{4\pi} \right)^2 \sum_{p=0}^\infty \int_1^\infty dx \ f(x) \int_0^\infty dt \int_0^\infty du \ \frac{\lambda_p^p}{p!} \ln^p \left( \frac{1+t}{tu} \right) \ \frac{1}{(1+t+u)^2}
\]

\[
\times \left\{ \frac{\tilde{k}^2}{(\tilde{k} + \tilde{a})^2} \ln \left( \frac{4\tilde{k}^2 x^2}{\tilde{a}^2} \right) + 2 \ \frac{\tilde{k}^2}{\tilde{a}^2 - \tilde{k}^2} \left[ 1 - \frac{2\tilde{k} \tilde{a}}{\tilde{a}^2 - \tilde{k}^2} \ln \left( \frac{\tilde{a}}{\tilde{k}} \right) \right] \right\}.
\]

(142)

To determine the corrections to the moments \( g_{n,1} \) we need the following inverse Laplace transforms [52], in addition to Eq. (135):

\[
\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \ \left[ \frac{2z^{2-p}}{A^2 - z^2} \right] e^{z^2n} = n^{\frac{p}{2} - 1} g_1(p, A^2 n),
\]

(143)

\[
\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \ \left[ - \frac{4Az^{3-p}}{(A^2 - z^2)^2} \right] e^{z^2n} = n^{\frac{p}{2} - 1} g_2(p, A^2 n),
\]

(144)

\[
41
\]
where
\[
g_1(p, X) \equiv -2 \left[ \frac{1}{\Gamma\left(\frac{\eta}{2}\right)} + e^X X^{1-\frac{p}{2}} \left( 1 - \frac{\Gamma\left(\frac{\eta}{2}, X\right)}{\Gamma\left(\frac{\eta}{2}\right)} \right) \right],
\]
\[
g_2(p, X) \equiv -2 \left[ \frac{2 \sqrt{X} (1 + X)}{\Gamma\left(\frac{1+p}{2}\right)} + e^X X^{1-\frac{p}{2}} (3 - p + 2X) \left( 1 - \frac{\Gamma\left(\frac{1+p}{2}, X\right)}{\Gamma\left(\frac{1+p}{2}\right)} \right) \right].
\]

The final result for the single insertion NNLO light quark mass corrections to the moments reads
\[
\left[ \delta g_{n,1}^{m,\text{NNLO}} \right]_{\text{single}} =
\]
\[
= 4 \sqrt{\pi} \left( \frac{a_s}{3 \pi} \right)^2 \phi \left\{ -\frac{3}{4} \int_1^\infty dx f(x) \left( h(x, n, \eta) \left( \beta_0 \ln \left( \frac{4m^2 x^2}{\mu^2} \right) - a_1 \right) + \beta_0 e^{\eta^2 x^2 n} \Gamma(0, \eta^2 x^2 n) \right) \\
+ \frac{3}{2} \sum_{p=1}^\infty \phi^p \left( \beta_0 \left( \ln \left( \frac{\mu^2}{m^2} \right) g_0(n, p, \eta) + g_2(n, p, \eta) \right) + a_1 g_0(n, p, \eta) \right) \\
+ 3 \beta_0 \left( \frac{1}{2} \ln^2 \left( \frac{c n \sqrt{\eta}}{2} \right) - \frac{5}{12} \ln \left( \frac{c n \sqrt{\eta}}{2} \right) + \frac{5 \pi^2}{48} \right) + \frac{3}{4} \left( \beta_0 \ln \left( \frac{\mu^2}{m^2} \right) + a_1 \right) \ln \left( \frac{c n \sqrt{\eta}}{2} \right) \\
- 3 \beta_0 \sum_{p=1}^\infty \phi^p \left( w^0_p \left( \operatorname{cln2}(n, p, \eta) + \frac{5}{6} \operatorname{cln}(n, p, \eta) + \frac{\pi^2}{12} \right) + 2 w^1_p \left( \operatorname{cln}(n, p, \eta) + \frac{5}{12} \right) - w^2_p \right) \\
+ \frac{3}{2} \left( \beta_0 \ln \left( \frac{\mu^2}{m^2} \right) + a_1 \right) \sum_{p=1}^\infty \phi^p \left( w^0_p \operatorname{cln}(n, p, \eta) + w^1_p \right) \right] \\
+ \left[ -\frac{1}{2} \int_1^\infty dx f(x) \left( h(x, n, \eta) \left( g(x) + \ln(4x^2) - \frac{5}{3} \right) + e^{\eta^2 x^2 n} \Gamma(0, \eta^2 x^2 n) \right) \\
+ \sum_{p=1}^\infty \phi^p \left( \varphi_1(n, p, \eta) + \varphi_2(n, p, \eta) + \frac{5}{3} \varphi_0(n, p, \eta) \right) \\
+ \frac{1}{2} \ln^2 \left( \frac{c n \sqrt{\eta}}{2} \right) + \frac{5 \pi^2}{48} - \sum_{p=1}^\infty \phi^p \left( w^0_p \left( \operatorname{cln2}(n, p, \eta) + \frac{\pi^2}{12} \right) + 2 w^1_p \operatorname{cln}(n, p, \eta) - w^2_p \right) \right] \\
+ \frac{57}{4} \left[ \frac{c_1}{2} \int_x^\infty dx h(x, n, \eta) + \frac{d_1}{2} \int_x^\infty dx h(x, n, \eta) + \sum_{p=1}^\infty \phi^p \varphi_3(n, p, \eta) \\
+ \frac{1}{2} \left( \ln \left( \frac{\eta \sqrt{n}}{2} \right) + \frac{c n}{2} + \frac{161}{228} + \frac{13}{19} \zeta_3 \right) \\
+ \sum_{p=1}^\infty \left( w^0_p \left( \frac{1}{2} \Psi \left( \frac{p}{2} \right) - \ln \left( \frac{\eta \sqrt{n}}{2} \right) - \frac{161}{228} - \frac{13}{19} \zeta_3 \right) + w^1_p \right) \right] \right},
\]

where
\[
c \equiv \exp \left( \frac{\gamma_E}{2} + \frac{5}{6} \right),
\]
\[
g(x) \equiv \frac{5}{3} + \frac{1}{x^2} \left( 1 + \frac{1}{2} \sqrt{x^2 - 1} (1 + 2x^2) \ln \left( \frac{x - \sqrt{x^2 - 1}}{x + \sqrt{x^2 - 1}} \right) \right),
\]

\[
h(x, n, \eta) \equiv e^{\eta^2 x^2 n} \left[ 1 - \text{erf}(\eta x \sqrt{n}) \right] = \frac{1}{\sqrt{\pi}} e^{\eta^2 x^2 n} \Gamma \left( \frac{1}{2}, \eta^2 x^2 n \right),
\]

\[
\text{cln}(n, p, \eta) \equiv \frac{1}{2} \Psi \left( \frac{p}{2} \right) - \ln \left( \frac{\eta \sqrt{n}}{2} \right) - \frac{5}{6},
\]

\[
\text{cln}^2(n, p, \eta) \equiv \left( \frac{1}{2} \Psi \left( \frac{p}{2} \right) - \ln \left( \frac{\eta \sqrt{n}}{2} \right) - \frac{5}{6} \right)^2 - \frac{1}{4} \Psi' \left( \frac{p}{2} \right),
\]

and

\[
\bar{g}_1(n, p, \eta) = -\int_0^\infty dt \int_0^\infty du \int_1^\infty dx f(x) \left[ \frac{5}{3} + \frac{1}{x^2} \left( 1 + \frac{1}{2} \sqrt{x^2 - 1} \right) \ln \left( \frac{x - \sqrt{x^2 - 1}}{x + \sqrt{x^2 - 1}} \right) \right] \\
\times \left. \frac{1}{p! (1 + t + u)^2} \ln^p \left( \frac{(1 + t) (1 + u)}{tu} \right) g_0(p, X) \right|_{X = \frac{\eta^2 x^2 n}{(1 + t + u)^2}},
\]

\[
\bar{g}_2(n, p, \eta) = -\int_0^\infty dt \int_0^\infty du \int_1^\infty dx f(x) \frac{1}{p! (1 + t + u)^2} \ln^p \left( \frac{(1 + t) (1 + u)}{tu} \right) \\
\times \left. \left( \ln \left( \frac{4 x^2}{X} \right) - 2 \frac{\partial}{\partial p} \right) g_0(p, X) + g_1(p, X) + \left( \frac{1}{2} \ln(X) + \frac{\partial}{\partial p} \right) g_2(p, X) \right|_{X = \frac{\eta^2 x^2 n}{(1 + t + u)^2}},
\]

\[
\bar{g}_3(n, p, \eta) = c_1 \int_0^\infty dt \int_0^{c_2} du \int_1^\infty dx \frac{1}{p! (1 + t + u)^2} \ln^p \left( \frac{(1 + t) (1 + u)}{tu} \right) g_0(p, X) \right|_{X = \frac{\eta^2 x^2 n}{(1 + t + u)^2}} \\
+ d_1 \int_0^\infty dt \int_0^\infty du \int_1^\infty dx \frac{1}{p! (1 + t + u)^2} \ln^p \left( \frac{(1 + t) (1 + u)}{tu} \right) g_0(p, X) \right|_{X = \frac{\eta^2 x^2 n}{(1 + t + u)^2}}.
\]

The constants \(w_p^0\), \(w_p^1\) and \(w_p^2\) have already been calculated in Ref. [7]; their expressions can be found in App. E. The three terms in the curly brackets on the RHS of Eq. (148) originate from the corresponding three terms given in Eq. (30), which all vanish individually for \(m \to 0\). If the \(\overline{\text{MS}}\) definition is used for the charm quark mass, \(m = m(\overline{m})[1 + \frac{4}{3}(a_s)]\), we get an additional contribution to the moments at NNLO through the replacement

\[
\delta q_{n,1}^{m,\text{NLO}}(n, \eta, a_s) \rightarrow \delta q_{n,1}^{m,\text{NLO}}(n, \eta, a_s) + \\
+ 32 \sqrt{\pi} \left( \frac{a_s}{3 \pi} \right)^2 \phi \left\{ \left[ - \frac{1}{2} \int_1^\infty dx f(x) \left( \frac{\eta x \sqrt{n}}{\sqrt{\pi}} - \eta^2 x^2 n h(x, n, \eta) \right) \right] + \sum_{p=1}^\infty \phi^p \bar{g}_4(n, p, \eta) \right\} \\
+ \left[ \frac{1}{4} - \frac{1}{2} \sum_{p=1}^\infty \phi^p w_p^0 \right],
\]

(157)
where
\[ \bar{\eta} = \frac{\bar{m}(\bar{m})}{M_b^{\text{pole}}} \],

and

\[ \bar{g}_4(n, p, \eta) = \int_0^\infty dt \int_0^\infty du \int_1^\infty dx f(x) \frac{1}{p!(1 + t + u)^2} \ln^p \left( \frac{(1 + t)(1 + u)}{tu} \right) \left[ X \frac{\partial}{\partial X} g_0(p, X) \right] \bigg|_{X = \frac{\eta^2 x^n}{(1 + t + u)^2}}. \]  

**(Light Quark Mass Corrections at NNLO – Double Insertions)**

The second and third terms on the RHS of Eq. (141) come from double insertions of the NLO static potential. The calculation of these contributions is much more involved than that of the ones coming from single insertions and will not be presented in this work. On the other hand, it is not necessary to include them in the present analysis. We have shown that the NNLO double-insertion contributions in the heavy quark pole–1S mass relation are suppressed with respect to the single-insertion ones; for the NNLO charm quark mass corrections, the double-insertion contributions amount to about 10% of the full NNLO result. As was pointed out in Sec. 4.2, this happens because at NNLO the corrections are dominated by momenta low enough for the linear (and \( r \)-independent) charm quark mass terms to dominate in the static potential. The same is expected for the double-insertion contributions of the NNLO charm quark mass corrections to the moments. Thus, the double-insertion contributions are of the same order as the terms \( \propto (m_{\text{charm}}/M_b)^n, n \geq 2 \), in the bottom quark pole–\( \overline{\text{MS}} \) mass relation, which are already neglected in this work. For the reasons mentioned here, we neglect the double-insertion contributions.

**Implementation of the 1S Mass**

The moments displayed in Eq. (128), including the charm quark mass corrections to \( \varrho_{n,1} \) in Eqs. (137) and (148), still depend on the bottom quark pole mass through the global factor \( (M_b^{\text{pole}})^{-2n} \) and through logarithms of ratios with the renormalization scales. The ratios of the pole mass with the renormalization scales originate from the running of the strong coupling and from anomalous dimensions of the \( 3S_1 \) NRQCD bottom quark currents. These ratios only arise at NLO and NNLO in \( \varrho_{n,1} \) and \( C_1 \). They do not lead to any modifications in the 1S mass scheme, because the difference between the bottom 1S and the pole masses is of order \( \nu^2 \sim \alpha_s^2 \sim 1/n \) in the non-relativistic power counting. The only relevant modification that arises from the implementation of the bottom 1S mass comes from the global factor \( (M_b^{\text{pole}})^{-2n} \). Using Eq. (79) and the scaling \( \alpha_s^2 \sim 1/n \), the global factor has the following form in the 1S mass scheme at NNLO in the non-relativistic expansion \( (a_s = \alpha_s^{(4)}(\mu_{\text{soft}})) \):

\[ \frac{1}{(M_b^{\text{pole}})^{2n}} = \frac{1}{(M_b^{1S})^{2n}} \exp \left( -2n \Delta_{\text{LO}}(a_s) \right) \]

\[ \times \left\{ 1 - 2n \left[ \Delta_{\text{massless}}^{\text{NLO}}(M_b^{1S}, a_s, \mu_{\text{soft}}) + \Delta_{\text{massive}}^{\text{NLO}}(\bar{m}(\bar{m}), M_b^{1S}, a_s) \right] \right. \]

\[ \left. + n \left( \Delta_{\text{LO}}^{\text{LO}}(a_s) \right)^2 + 2n \left( \Delta_{\text{massless}}^{\text{NLO}}(M_b^{1S}, a_s, \mu_{\text{soft}}) + \Delta_{\text{massive}}^{\text{NLO}}(\bar{m}(\bar{m}), M_b^{1S}, a_s) \right)^2 \right\} \]
\[
-2 \left( \Delta_{\text{massless}}^{\text{NNLO}}(M_{b}^{1S}, a_{s}, \mu_{\text{soft}}) + \Delta_{\text{massive}}^{\text{NNLO}}(m/m, M_{b}^{1S}, a_{s}, \mu_{\text{soft}}) \right) \\
-2 \delta^{(1)}(a_{s}) \Delta_{m}^{\text{NLO}}(m/m, M_{b}^{1S}, a_{s}) \right) \rightbrace, \tag{160}
\]

where the \( \Delta \)'s have been given in Eqs. (35), (54)–(56), (63), (64) and (78). The second and third terms in the curly brackets on the RHS of Eq. (160) are the NLO and NNLO contributions, respectively. We emphasize that using Eq. (160) for the global factor \( 1/(M_{b}^{\text{pole}})^{2n} \) in Eq. (128) is equivalent to implementing the bottom 1S mass via Eq. (79) into the Schrödinger equation (1) before any calculation is carried out. The renormalization scale on the RHS of Eq. (160) is \( \mu_{\text{soft}} \), which governs the strong coupling in the static potential. This is because the corrections on the RHS of Eq. (160) only involve non-relativistic momenta. From the technical point of view, they are supposed to compensate for the bad large order behaviour of the static potential. For the same reason we have to consistently expand the LO, NLO and NNLO corrections in Eq. (160) with the LO, NLO and NNLO corrections in \( \varrho_{n,1} \).

Aside from the issue of the cancellation of the large high order corrections that are associated with the bottom quark pole mass definition, it is easy to understand how the 1S mass definition reduces the correlation of the moments (and also of the mass determination) to the strong coupling and the dependence on \( \mu_{\text{soft}} \): in the 1S scheme the exponential energy-enhancement of the \( {^3S_1} \) bottom–antibottom ground state that dominates the moments for large values of \( n \), is eliminated. A detailed discussion of this effect has been given in Ref. [9].

**Light Quark Mass Corrections to the Short-Distance Coefficient \( C_{1} \)**

The short-distance coefficient \( C_{1} \) contains the effects of the bottom–antibottom quark production process that arise from momenta of order \( M_{b} \). This has two consequences: the first is that the light quark mass corrections can be naively expanded in \( m^{2} \) without the emergence of any terms that are non-analytic in \( m^{2} \). Thus, \( C_{1} \) does not contain any linear dependence on a light quark mass. The second consequence is that one can expand in the light quark mass because \( m/M_{b} \) is small. Therefore, the dominant light quark mass effect in \( C_{1} \) is proportional to \( (\alpha_{s}/\pi)^2(m/M_{b})^2 \), where the scale in the strong coupling is of order \( M_{b} \). For the charm quark this correction is at the per mille level and subleading. The charm mass corrections to \( C_{1} \) are of the same order as the \( m^{2}/M_{c} \) corrections in the pole–\( \overline{\text{MS}} \) mass relation that have been neglected in this work. The light quark mass corrections to \( C_{1} \) are therefore also neglected in this work. We note that the absence of any linear light quark mass corrections in \( C_{1} \) has been proved by explicit calculation in Ref. [53]. It was shown, for any energy at order \( \alpha_{s}^2 \), that the total cross section \( R \), Eq. (107), does not contain any linear light quark mass corrections if a short-distance definition is employed for the bottom quark mass. Thus, because \( C_{1} = 1 \) (and is mass independent) at the Born approximation, it cannot contain linear light quark mass corrections at order \( \alpha_{s}^2 \).

**6.4 Brief Examination**

Before turning to the statistical analysis it is useful to examine the size and behaviour of the light quark mass corrections to the moments for various choices of the light quark mass. This will be helpful for the interpretation of the result that is obtained for the bottom 1S mass from the sum rule analysis carried out in the next section. Detailed discussions on the behaviour of the moments in the pole and the 1S mass schemes for the case of massless light quarks can be found in Refs. [7, 9].
any of the detailed discussions of Ref. [9].

Therefore we do not repeat observations for the behaviour of the moments in the 1S mass scheme made in the analysis of Ref. [9] for the determination of the bottom mass $m_b$. This can be estimated from the overall mass dependence of the moments, see for instance Eqs. (108) and (113). We will see in Sec. 7 that this is indeed the case. Interestingly, the NNLO light quark mass corrections are actually larger than the NLO ones and their effects in the perturbative bottom–antibottom 1S wave function at the origin that were determined for the $\mu$ values for $\mathcal{O}(\alpha_s^4) (M_Z)$, this means that the charm mass corrections remain qualitatively true if the effects of light quark masses are included. Therefore we do not repeat any of the detailed discussions of Ref. [9].

In Table 7 the values of $P_n^{th}$ at LO, NLO and NNLO have been displayed for $M_b^{1S} = 4.7$ GeV, $\alpha_s^{(4)} (M_Z) = 0.118$, $\mu_{\text{soft}} = 2.5$ GeV and $\mu_{\text{hard}} = \mu_{\text{fac}} = 5$ GeV, for various values of $\overline{m}(\overline{m})$ and $n = 4, 6, 8, 10, 20$. The values for $P_n^{th}$ for $\overline{m}(\overline{m}) = 0.0$ GeV are slightly different from the numbers shown in Ref. [9] as we used four-loop running and three-loop matching conditions at the five-four flavour threshold for the determination of strong coupling at the lower scales. In Ref. [9] two-loop running was employed.

<table>
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<tr>
<th>$\overline{m}(\overline{m})$ [GeV]</th>
<th>0.0</th>
<th>0.1</th>
<th>1.0</th>
<th>1.5</th>
<th>2.0</th>
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<tr>
<td>$P_n^{th,\text{LO}} [10^8 \text{ GeV}^8]$</td>
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<tr>
<td>$P_n^{th,\text{NNLO}} [10^8 \text{ GeV}^8]$</td>
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<td>0.231</td>
<td>0.231</td>
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<tr>
<td>$P_n^{th,\text{LO}} [10^{12} \text{ GeV}^{12}]$</td>
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<td>0.268</td>
<td>0.268</td>
<td>0.268</td>
<td>0.268</td>
</tr>
<tr>
<td>$P_n^{th,\text{NLO}} [10^{12} \text{ GeV}^{12}]$</td>
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<td>0.145</td>
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<tr>
<td>$P_n^{th,\text{NNLO}} [10^{12} \text{ GeV}^{12}]$</td>
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<td>$P_n^{th,\text{NLO}} [10^{16} \text{ GeV}^{16}]$</td>
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<td>0.617</td>
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Table 7: The theoretical moments $P_n^{th}$ at LO, NLO and NNLO for $M_b^{1S} = 4.7$ GeV, $\alpha_s^{(4)} (M_Z) = 0.118$, $\mu_{\text{soft}} = 2.5$ GeV and $\mu_{\text{hard}} = \mu_{\text{fac}} = 5$ GeV, for various values of $\overline{m}(\overline{m})$ and $n = 4, 6, 8, 10, 20$. The values for $P_n^{th}$ for $\overline{m}(\overline{m}) = 0.0$ GeV are slightly different from the numbers shown in Ref. [9] as we used four-loop running and three-loop matching conditions at the five-four flavour threshold for the determination of strong coupling at the lower scales. In Ref. [9] two-loop running was employed.

Let us first discuss the results for $n \leq 10$. The numbers show that the light quark mass corrections are positive at NLO and negative at NNLO. (The observation that the NLO light quark mass corrections to the moments are positive is consistent with the NLO results for the charm quark mass effects in the perturbative bottom–antibottom 1S wave function at the origin that were determined in Ref. [54].) The NNLO light quark mass corrections are actually larger than the NLO ones and lead to an overall negative shift in the moments at NNLO. For $n = 4$ the overall shift is around $-1\%$ and for $n = 10$ around $-5\%$, for $\overline{m}(\overline{m}) \approx 1.5$ GeV. This means that the bottom 1S mass that is extracted from the $\Upsilon$ sum rule analysis receives a negative shift of the order of 15 MeV from the charm mass effects. This can be estimated from the overall mass dependence of the moments, see for instance Eqs. (108) and (113). We will see in Sec. 7 that this is indeed the case. Interestingly, for the determination of the bottom $\overline{\Sigma}$ mass $\overline{M}_b(\overline{M}_b)$, this means that the charm mass corrections
in the moments of the Υ sum rules and in the $\overline{\text{MS}}$–1S mass relation are additive. The fact that the NNLO light quark corrections are larger than the NLO ones and lead to an overcompensation is not necessarily a point of concern, because the light quark mass corrections should be viewed as a part of the full corrections. Their behaviour is essentially not affected by that due to the small overall size of the light quark mass corrections. Nevertheless, one can and should ask why the behaviour of the light quark mass corrections in the moments is so much worse than in the bottom $\overline{\text{MS}}$–1S mass relation discussed in Sec. 5. To judge the situation properly, however, one also has to take into account that the convergence of the massless corrections is also much worse in the moments than in the bottom $\overline{\text{MS}}$–1S mass relation. (Compare the numbers shown in Table 5 with those in Table 7.) The difference in the behaviour of the perturbative series comes from the fact that the moments also depend on the square of the bottom–antibottom wave function at the origin (through their dependence on the bottom–antibottom decay and production rate). It is well known that the non-relativistic expansion of the bound state wave function at the origin is much worse than for the binding energy. A complete theoretical understanding of the physical origin of this behaviour, which could subsequently lead to an improvement of the situation, has not been achieved yet. However, it seems obvious that the problem arises from the infrared region\(^9\). Paradoxically, the wave function at the origin is not affected by the question of the quark mass definition, which is generally argued to represent the dominant issue as far as infrared sensitivity is concerned; whether we use the bottom 1S mass or the bottom pole mass does essentially not affect corrections to the wave function as shifts to the energy in the Schrödinger equation (1) leave the wave function unchanged. The behaviour of the light quark mass corrections in the moments therefore seems to be just a reflection of the present situation, in particular because the light quark mass corrections are, as mentioned several times earlier, very sensitive to moments smaller than the light quark mass. The present situation is that the moments of the Υ sum rules have a perturbative expansion that is much worse than the perturbative expansion of the bottom $\overline{\text{MS}}$–1S mass relation, although general arguments based on global duality tell that the infrared sensitivity of the moments should be smaller \([45]\), and although the gluon condensate contributions to the moments are negligibly small compared to the ones in the Υ(1S) mass. For the fits that we carry out in Sec. 7 to determine the bottom 1S mass, we will disregard this problem as was done in previous Υ sum rule analyses.

Let us now discuss the results for $n = 20$. We emphasize that moments $P_n$ for $n > 10$ are not employed in our analysis. The light quark mass corrections for $m(m) \approx 1.5$ GeV at NLO and NNLO are scaringly large individually (of the order of 50% of the full corrections in each order), but lead to a relatively moderate overall correction at NNLO (of the order of 15%). We cannot exclude that, for very large values of $n$, the neglected double-insertion contributions at NNLO are very strongly enhanced for some reason, but we believe that this is very unlikely. The behaviour of the light quark mass corrections to the moments at very large values of $n$ therefore seem to reflect the increased infrared sensitivity of the moments if $n$ is considerably larger than 10. This is in agreement with the general considerations made by Poggio, Quinn and Weinberg \([45]\) about the required minimal size of the energy interval in the integration that defines the moments in Eq. (106). Thus the use of moments with $n$ much larger than 10 could potentially lead to large systematic uncertainties and should be avoided.

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\(^9\)Voloshin \([55]\) (see also Ref. \([56]\)) made the observation that the relative gluon condensate correction is about three times larger for the square of the wave functions at the origin than for the energy levels.
Determination of the Bottom Mass from the $\Upsilon$ Sum Rules

In this section we carry out the numerical analysis for the determination of the bottom quark 1S and $\overline{\text{MS}}$ masses using the $\Upsilon$ sum rules. In the analysis we put the main focus on the effects coming from the finite charm quark mass. In the previous sections the effects of the up, down and strange quark masses have shown to be negligible. They are not included in the analysis. In Sec. 7.1 we will briefly review the statistical procedure that is used in the sum rule analysis, and in Sec. 7.2 we show the results for the bottom quark 1S mass. In Sec. 7.3 the results for the bottom quark 1S mass are confronted with the mass of the $\Upsilon(1S)$ and the implications for non-perturbative corrections in the $\Upsilon(1S)$ mass are examined. In Sec. 7.4 the bottom $\overline{\text{MS}}$ mass is derived from the 1S mass result.

7.1 Statistical Procedure

To obtain numerical results for the 1S mass we use a statistical procedure based on the $\chi^2$-function

$$
\chi^2(M_{b}^{1S}, \alpha_s^{(5)}(M_Z), \mu_{\text{soft}}, \mu_{\text{hard}}, \mu_{\text{fac}}) = \sum_{\{n\},\{m\}} (P_n^{\text{th}} - P_n^{\text{ex}}) (S^{-1})_{nm} (P_m^{\text{th}} - P_m^{\text{ex}}),
$$

where $\{n\}$ represents the set of $n$’s for which the fit is carried out and $S^{-1}$ is the inverse covariance matrix describing the experimental errors and the correlation between the experimental moments. (See Ref. [7] for a detailed description of the covariance matrix.) We emphasize that the renormalization scale dependence of the theoretical moments implemented in $\chi^2$ is exactly as displayed in the formulae in Secs. 6.2 and 6.3 and that no optimization procedure has been carried out. The covariance matrix contains the errors in the $\Upsilon$ electronic decay widths, the electromagnetic coupling $\tilde{\alpha}_{\text{em}}$, and the continuum cross section $r_{\text{cont}}$. The small errors in the $\Upsilon$ masses are neglected. The correlations between the individual measurements of the electronic decay widths are estimated to be equal to the product of the respective systematic errors given in Table 6. In our two previous analyses in Refs. [7, 9] we have varied the correlation between this product and zero, and we found that the results are insensitive to this choice. In order to estimate the theoretical uncertainties in the mass extraction, the renormalization scales $\mu_{\text{soft}}, \mu_{\text{hard}}$ and $\mu_{\text{fac}}$ are varied randomly in the ranges

$$
1.5 \text{ GeV} \leq \mu_{\text{soft}} \leq 3.5 \text{ GeV},
$$
$$
2.5 \text{ GeV} \leq \mu_{\text{hard}} \leq 10 \text{ GeV},
$$
$$
2.5 \text{ GeV} \leq \mu_{\text{fac}} \leq 10 \text{ GeV},
$$

and the following sets of $n$’s

$$
\{n\} = \{4, 5, 6, 7\}, \{7, 8, 9, 10\}, \{4, 6, 8, 10\}
$$

are employed. Because the strong coupling cannot be extracted from the sum rules based on the $\chi^2$ function in Eq. (161) with relative uncertainties smaller than 10% (see the corresponding results of Refs. [7, 9]) we fit $M_b^{1S}$, taking $\alpha_s^{(5)}(M_Z)$ as an input\(^\text{10}\). For each choice of the renormalization scales

\(^{10}\text{For this work we have also carried out a simultaneous fit of } M_b^{1S} \text{ and } \alpha_s^{(5)}(M_Z). \text{ The results are not discussed in this work. As in the previous analyses in Refs. [7, 9] we found a relative uncertainty of 10% in } \alpha_s^{(5)}(M_Z). \text{ The results for } M_b^{1S} \text{ were found to be equivalent to those obtained when } \alpha_s^{(5)}(M_Z) \text{ is taken as an input.}\)
μ_{soft}, μ_{hard}, μ_{fac} in the ranges (162), each set of n’s and each given value of α_s^{(5)}(M_Z), M_b^{1S} is obtained for which χ^2 is minimal.

We note that the dependence of the theoretical moments on variations of the renormalization scales, and in particular of μ_{soft}, is rather large, see Table 3 of Ref. [9]. This strong dependence is a reflection of the bad convergence properties of the moments caused by their dependence on the square of the bottom–antibottom wave functions at the origin, which we have already discussed in Sec. 6.4. It turns out that the χ^2-function in Eq. (161) has a smaller renormalization scale dependence than the individual moments, because it puts higher weight on linear combinations of the moments (P^n – P^n_{ex}) for which the overall dependence on μ_{soft} in the wave functions partially cancels. This feature arises from the fact that the scale sensitivity of the squared wave functions for low radial bottom–antibottom excitations roughly corresponds to the size and correlation of the experimental uncertainties of the respective electronic Υ decay rates. Since the inverse covariance matrix puts higher weight on those linear combinations of the moments (P^n – P^n_{ex}) for which the experimental uncertainties coming from the electronic decay widths cancel, this consequently leads to partial cancellation of the scale dependence. This means that the χ^2-function essentially fits the relative size of the moments (as a function of n for a given value of μ_{soft}) and not so much their overall normalization. In particular, this means that the resulting estimate for the theoretical uncertainty in the bottom 1S mass based on the χ^2-function in Eq. (161) is smaller than an estimate that is only based on a single moment. The estimate based on the χ^2-function is more realistic if the true theoretical uncertainties of the moments (and of the squared wave functions at the origin for the low radial excitations in particular), which are arising from truncating the perturbative series, are correlated according to their scale dependence. The stability of the estimate for the bottom 1S mass based on the χ^2-function in Eq. (161) under inclusion of higher order perturbative corrections (see Figs. 5 and 6 in Sec. 7.2) seems to support that this is the case.

### 7.2 Results for the Bottom 1S Mass

In Figs. 5 and 6, the allowed range for the bottom 1S mass is displayed as a function of the strong coupling based on the NLO and NNLO theoretical moments, respectively, for the charm MS masses \( \overline{m}(\overline{m}) = 1.1, 1.3, 1.5 \) and 1.7 GeV. As a comparison, the results for \( \overline{m}(\overline{m}) = 0.0 \) and 0.15 GeV are also shown. Each dot represents the bottom 1S mass for which the function χ^2 is minimal for given (random) values of α_s and the renormalization scales and a given set of n’s. For the running of the strong coupling we employed the four-loop beta function and three-loop matching conditions at the five-four flavour threshold. The experimental and statistical errors that are indicated by the vertical lines correspond to 95% CL. They are below 15 MeV for all dots displayed in Figs. 5 and 6. We note that the NNLO results do not depend on whether the NNLO double-insertion charm mass corrections in the relation between the bottom pole and 1S masses in Eq. (160) are taken into account or not.

Figures 5 show that at NLO the inclusion of the finite charm mass does not at all affect the results for the bottom 1S mass. For all choices of the MS charm quark mass between 1.1 and 1.7 GeV the allowed range for \( M_b^{1S} \) is practically identical to the analysis where the charm mass is neglected. Assuming

\[
α_s^{(5)}(M_Z) = 0.118 \pm 0.003
\]  

(164)

for the strong coupling, which is motivated by the compilations given in Refs. [57, 58], we arrive at
Figure 5: Results for the allowed range of $M_{b}^{1S}$ for given values of $\alpha_{s}^{(5)}(M_{Z})$ (and the corresponding values of $\alpha_{s}^{(4)}(2.5\,\text{GeV})$) at NLO for different choices of the \MS charm quark mass. The dots represent points of minimal $\chi^2$ for a large number of random choices within the ranges (162) and the sets (163), and randomly chosen values of the strong coupling. Experimental errors at 95% CL are displayed as vertical lines. It is illustrated how the allowed range for $M_{b}^{1S}$ is obtained if $0.115 \leq \alpha_{s}^{(5)}(M_{Z}) \leq 0.121$ is taken as an input.

$M_{b}^{1S} = 4.70 \pm 0.06$ GeV from the fits to the NLO theoretical moments. Although we assume a smaller uncertainty for $\alpha_{s}$ than in our previous analysis of Ref. [9], where we used $\alpha_{s}^{(5)}(M_{Z}) = 0.118 \pm 0.004$, the result for the bottom 1S mass is equivalent to the one obtained at NLO in Ref. [9]. This is because the correlation of the allowed range for the 1S mass to the value of the strong coupling is rather weak.
Figure 6: Results for the allowed range of $M_{b}^{1S}$ for given values of $\alpha_s^{(5)}(M_{Z})$ (and the corresponding values of $\alpha_s^{(5)}(2.5 \text{ GeV})$) at NNLO for different choices of the MS charm quark mass. The dots represent points of minimal $\chi^2$ for a large number of random choices within the ranges (162) and the sets (163), and randomly chosen values of the strong coupling. Experimental errors at 95% CL are displayed as vertical lines. It is illustrated how the allowed range for $M_{b}^{1S}$ is obtained if $0.115 \leq \alpha_s^{(5)}(M_{Z}) \leq 0.121$ is taken as an input.

(and because we round the results to 10 MeV precision). In contrast to the NLO results shown in Ref. [9], Fig. 5 exhibits an instability in the allowed 1S mass range for input values of $\alpha_s^{(5)}(M_{Z})$ larger than 0.125. This is caused by the use of the four-loop running for the strong coupling, which leads to larger values of $\alpha_s$ at lower scales than the two-loop running that has been used in Ref. [9]. For the
extraction of the bottom 1S mass using Eq. (164) as an input, this instability is irrelevant.

Figures 6 show the results for the allowed bottom 1S mass range obtained from the NNLO theoretical moments. The results have a number of remarkable features. Most prominently, the already weak correlation of the allowed bottom 1S mass range with the strong coupling visible in the NLO analysis has completely vanished in the relevant strong coupling range \( \alpha_s(M_Z) \approx 0.118 \) if the effects of the charm quark mass are included. This leads to a variation of the bottom 1S mass slightly smaller than the analysis with zero charm quark mass. We also find that the central value for the bottom 1S mass is about 20 MeV lower if the charm quark mass is taken into account. Taking Eq. (164) as an input we arrive at

\[
M_{1S}^b = 4.69 \pm 0.03 \text{ GeV}
\]  

(165)

for the bottom 1S mass from the NNLO theoretical moments, taking into account the charm \( \overline{\text{MS}} \) mass \( m(\overline{m}) = 1.4 \pm 0.3 \text{ GeV} \). We emphasize that the uncertainty of 30 MeV in Eq. (165) does not depend at all on the uncertainty of the strong coupling. It is also interesting that the allowed range for the bottom 1S mass is stabilized for \( \alpha_s(M_Z) \) larger than 0.125 compared to the NLO analysis. We note that the fact that the bottom 1S mass gets a negative shift from the finite charm quark mass is expected, because a light quark mass gives negative corrections to the NNLO theoretical moments (see the discussion in Sec. 6.4). Neglecting the charm quark mass, the result reads \( M_{1S}^b = 4.71 \pm 0.04 \text{ GeV} \), where the variation is slightly larger than in Ref. [9] owing to the use of the four-loop beta function for \( \alpha_s \).

7.3 Comparison with the Mass of the \( \Upsilon(1S) \) Meson

It is a quite interesting feature of our NNLO result for the bottom 1S mass, \( M_{1S}^b = 4.69 \pm 0.03 \text{ GeV} \), that it could be used to constrain the non-perturbative effects in the mass of the \( \Upsilon(1S) \) meson, \( M(\Upsilon(1S)) = 9460.37 \pm 0.21 \text{ MeV} \). We remind the reader that, because we only used moments \( P_n \) with \( n \leq 10 \), the bottom–antibottom quark dynamics in the sum rules can be treated as perturbative (i.e. that the hierarchy “\( M_b \gg M_b v \gg M_s v^2 \gg \Lambda_{\text{QCD}} \)” is satisfied). Thus, non-perturbative corrections to the moments can be reliably determined in an expansion in gluonic and light quark condensates of increasing dimensions.\(^\text{11}\) For the moments \( P_n \) with \( n \leq 10 \) the dominant non-perturbative corrections from the dimension-4 gluon condensate corrections are below the per mille level (see Eq. (110)). We therefore assume that non-perturbative effects in general can be safely neglected in our sum rule analysis. This means that our result for the bottom 1S mass in Eq. (165) is not affected at all by non-perturbative effects. On the other hand, the bottom quark 1S mass is just half of the perturbative contribution of the mass of the \( \Upsilon(1S) \) meson, assuming that the latter is also a perturbative system.

If we assume that the \( \Upsilon(1S) \) meson can be treated as a perturbative system (at least as far as the calculation of its mass is concerned), non-perturbative corrections in \( M(\Upsilon(1S)) \) can also be reliably determined in an expansion in the condensates. However, the corrections caused by the condensates are much larger than for the sum rules and cannot be neglected as in the sum rule analysis. A precise and accurate determination of the bottom 1S mass from the \( \Upsilon \) sum rules could therefore be used to seriously test the hypothesis that the \( \Upsilon(1S) \) is perturbative and, eventually, to extract more precise

\(^\text{11}\)We assume for now that the expansion in terms of condensates is valid for the moments if \( n \) is not too large, and disregard the discussions in Secs. 6.1 and 6.4.
values for the condensates. From the NNLO sum rule result for the bottom 1S mass in Eq. (165), we find

\[
M(\Upsilon(1S))_{\text{non-pert}} = M(\Upsilon(1S)) - 2M_{b}^{1S} = 80 \pm 60 \text{ MeV}
\]  

(166)

for the non-perturbative contributions in the \(\Upsilon(1S)\) mass. We emphasize again that the result in Eq. (166) can only be interpreted as “the non-perturbative contributions in the \(\Upsilon(1S)\) mass” based on the hypothesis that the \(\Upsilon(1S)\) is a perturbative system. It is interesting that Eq. (166) seems indeed consistent with the leading dimension-four gluon condensate contribution obtained by Voloshin and Leutwyler [55, 56]:

\[
M(\Upsilon(1S))_{\text{non-pert}} = \frac{1872}{1275} M_{b} n^{6} \pi \langle \alpha_{s} G^{2} \rangle_{\Lambda_{\text{QCD}}} + \ldots .
\]  

(167)

Equation (167) obtains corrections from higher-dimension condensates as well as higher order perturbative corrections to the Wilson coefficients multiplying each of the condensates. The subleading dimension-6 condensate contributions have been calculated in Ref. [59]. The unknown perturbative corrections induce a very large scale uncertainty of the dimension-4 condensate contribution shown in Eq. (167). Assuming the standard literature range \(\langle \alpha_{s} G^{2} \rangle_{\Lambda_{\text{QCD}}} = 0.05 \pm 0.03 \text{ GeV}^{4}\) the leading gluon condensate correction can range from 10 up to 300 MeV (for \(0.2 < \alpha_{s} < 0.5\)), where large numbers paradoxically correspond to smaller values of the strong coupling. As said before, this range is consistent with Eq. (166), but at the present stage it does not provide any meaningful determination of \(\langle \alpha_{s} G^{2} \rangle\), let alone a test of the hypothesis that the \(\Upsilon(1S)\) is perturbative. The calculation of higher order perturbative corrections in Eq. (167) would be very helpful to clarify the situation.

### 7.4 Results for the Bottom \(\overline{\text{MS}}\) Mass

The heavy quark 1S mass is, by design, a short-distance mass adapted to systems where the heavy quark is very close to its mass shell, or, in other word, where the heavy quark virtuality is much smaller than its mass, \(q^{2} - M_{Q}^{2} \ll M_{Q}^{2}\). Apart from heavy-quark–antiquark systems the 1S mass definition has also been applied to B mesons [20], where the bottom quark virtuality is of order \(\Lambda_{\text{QCD}} M_{Q}\). For high-energy or low-energy processes, however, where the heavy quark virtuality is of order \(M_{Q}^{2}\) or larger, the \(\overline{\text{MS}}\) mass definition is the preferred one. In this section we determine the bottom \(\overline{\text{MS}}\) mass from the NNLO result for the 1S mass in Eq. (165) using formula (82).

In Figs. 7 the dependence of the bottom \(\overline{\text{MS}}\) mass \(M_{b}(\overline{M}_{b})\) on the charm quark \(\overline{\text{MS}}\) mass \(\overline{m}(\overline{m})\), the strong coupling \(\alpha_{s}^{(5)}(M_{Z})\), the renormalization scale \(\mu\) (of the strong coupling entering the relation between the bottom \(\overline{\text{MS}}\) and 1S masses) and the bottom 1S mass \(M_{b}^{1S}\) is displayed. In each plot the respective fixed parameters have been chosen as \(\alpha_{s}^{(5)}(M_{Z}) = 0.118\), \(M_{b}^{1S} = 4.69 \text{ GeV}\) and \(\mu = 4.69 \text{ GeV}\), if not stated otherwise. Figure 7a shows \(\overline{M}_{b}(\overline{M}_{b})\) as a function of the charm mass for \(\mu = 6.7 \) (dashed line), 4.69 (solid line) and 2.7 GeV (dotted line). Figures 7b,c,d show \(\overline{M}_{b}(\overline{M}_{b})\) as a function of \(\mu\), \(M_{b}^{1S}\) and \(\alpha_{s}^{(5)}(M_{Z})\) for \(\overline{m}(\overline{m}) = 0.0 \text{ GeV}\) (solid lines), 1.1 GeV (dotted lines), 1.3 GeV (dash-dotted lines), 1.5 GeV (dashed lines) and 1.7 GeV (long-dashed lines). It is conspicuous that for \(\overline{m}(\overline{m}) > 0.4 \text{ GeV}\) and \(\mu \gtrsim 2.5 \text{ GeV}\) the dependence of \(\overline{M}_{b}(\overline{M}_{b})\) on all four parameters is approximately linear. This welcome feature allows for the derivation of the following handy approximation formula:

\[
\overline{M}_{b}(\overline{M}_{b}) = 4.169 \text{ GeV} - 0.01 \left(\overline{m}(\overline{m}) - 1.4 \text{ GeV}\right) + 0.925 \left(M_{b}^{1S} - 4.69 \text{ GeV}\right)
\]
Figure 7: The dependence of the bottom \( \overline{\text{MS}} \) mass \( \overline{M}_b(M_b) \), determined from the bottom 1S mass, on the \( \overline{\text{MS}} \) charm quark mass (a), the renormalization scale \( \mu \) (b), the bottom 1S mass \( M^{1S}_b \) (c) and the strong coupling \( \alpha_s^{(5)}(M_Z) \) (d). In each plot the fixed parameters have been chosen as \( \alpha_s^{(5)}(M_Z) = 0.118 \), \( M^{1S}_b = 4.69 \) GeV and \( \mu = 4.69 \) GeV, if not stated otherwise. In (a) the result is displayed for \( \mu = 6.7 \) (dashed line), 4.69 (solid line) and 2.7 GeV (dotted line). In (b,c,d) the result is displayed for \( m(m) = 0 \) GeV (solid lines), 1.1 GeV (dotted lines), 1.3 GeV (dash-dotted lines), 1.5 GeV (dashed lines) and 1.7 GeV (long-dashed lines).

\[
-9.1\left(\alpha_s^{(5)}(M_Z) - 0.118\right) \text{GeV} + 0.0057 \left(\mu - 4.69\right) \text{GeV}, \tag{168}
\]

For \( m(m) > 0.4 \) GeV and \( \mu > 2.5 \) GeV the difference between this approximation formula and the exact result is less than 3 MeV. Figures 7 and Eq. (168) show that at present the dominant uncertainties arise from the errors in the strong coupling and the bottom quark 1S mass. The error in \( \overline{M}_b(M_b) \) induced by \( M^{1S}_b \) is roughly equal to the error in \( M^{1S}_b \), and the one induced by \( \alpha_s \) roughly amounts to \( x \) times 10 MeV for an uncertainty of \( x \) times 0.001 in \( \alpha_s^{(5)}(M_Z) \). At the present stage \( M^{1S}_b \) and \( \alpha_s^{(5)}(M_Z) \) each contribute about 30 MeV to the uncertainty of \( \overline{M}_b(M_b) \). The uncertainty coming from the scale variation and from the error in the charm mass corrections, which arises from the uncertainty in \( m(m) \) and the neglected order \( m^2/M_b \) corrections in the bottom pole–\( \overline{\text{MS}} \) mass relation, is much smaller. Varying the renormalization scale by 1 GeV shifts \( \overline{M}_b(M_b) \) by about 5 MeV. This variation reflects the remaining perturbative uncertainty contained in the order \( \alpha_s^2 \) relation between the bottom \( \overline{\text{MS}} \) and 1S masses. We assign a perturbative uncertainty based on a 3 GeV variation of the renormalization scale.
which gives 15 MeV. We estimate the error in the charm mass corrections as 5 MeV, which includes
the sources of uncertainties in the charm mass corrections mentioned before and mass corrections
coming from the other light quarks. Adding all uncertainties quadratically, we obtain

$$
\bar{M}_b(\bar{M}_b) = 4.17 \pm 0.05 \text{ GeV},
$$

(169)

where the central value has been determined for $M_b^{1S} = \mu = 4.69 \text{ GeV}$, $\alpha_s^{(5)}(M_Z) = 0.118$ and $\overline{\text{m}}(\overline{\text{m}}) = 1.4 \text{ GeV}$. The result is rounded to units of 10 MeV.

It is instructive to compare the result with the one obtained if the charm quark mass were
neglected entirely: starting from $4.71 \pm 0.04 \text{ GeV}$ for the bottom 1S mass we would arrive at $\bar{M}_b(\bar{M}_b) = 4.20 \text{ GeV} \pm 30 \text{ MeV} [\delta \alpha_s] \pm 40 \text{ MeV} [\delta M_b^{1S}] \pm 15 \text{ MeV} [\mu] = 4.20 \pm 0.05 \text{ GeV}$, where the central value is
obtained for $M_b^{1S} = \mu = 4.71 \text{ GeV}$ and $\alpha_s^{(5)}(M_Z) = 0.118$. Thus, after rounding to units of 10 MeV,
the overall effect of the finite charm quark mass on the bottom $\overline{\text{MS}}$ mass is a shift of $-30 \text{ MeV}$.

Let us briefly comment on the results for $\bar{M}_b(\bar{M}_b)$ that we gave in Refs. [9, 38], where the
bottom 1S mass was also used as an intermediate step to determine $\bar{M}_b(\bar{M}_b)$, but where charm mass
effects were neglected. In Ref. [9] we have obtained $\bar{M}_b(\bar{M}_b) = 4.20 \pm 0.06 \text{ GeV}$. The central value
was obtained for $M_b^{1S} = \mu = 4.71 \text{ GeV}$ and $\alpha_s^{(5)}(M_Z) = 0.118$, not using formula (82) for $\overline{\text{m}}(\overline{\text{m}}) = 0$, but solving Eqs. (34) and (53) numerically for a given value of $M_b^{1S}$. The order $\alpha_s^3$ terms were not
included because at that time the order $\alpha_s^3$ corrections in the pole-$\overline{\text{MS}}$ mass relation [12, 35] where
not yet known. The agreement of the central value with the one mentioned in the previous paragraph
is a coincidence. The 60 MeV uncertainty was estimated by assuming a 40 MeV perturbative error, a
40 MeV error caused by the strong coupling (assuming $\alpha_s^{(5)}(M_Z) = 0.118 \pm 0.004$) and a 30 MeV error
for $M_b^{1S}$. The result $\bar{M}_b(\bar{M}_b) = 4.21 \pm 0.07 \text{ GeV}$ in the proceedings quoted in Ref. [38] was obtained
from formula (82) for $\overline{\text{m}}(\overline{\text{m}}) = 0$, assuming $M_b^{1S} = 4.73 \pm 0.05 \text{ GeV}$, $\mu = 4.73 \text{ GeV}$ and $\alpha_s^{(5)}(M_Z) = 0.118 \pm 0.004$. The value for the bottom 1S mass was determined from $M_b^{1S} = 1/2(M_\Upsilon(1S) + \Delta_{\text{non-pert}})$
assuming $\Delta_\Upsilon(1S) \approx 100 \text{ MeV}$ for the non-perturbative contribution in the $\Upsilon(1S)$ mass. After rounding
to units of 10 MeV, the error was 10 MeV larger than the one obtained from formula (82) (for $\overline{\text{m}}(\overline{\text{m}}) = 0$) used in this work because in Ref. [38] the corresponding formula was based on the numerical
order $\alpha_s^3$ corrections to the pole-$\overline{\text{MS}}$ mass relation from Ref. [35]. Equation (82), on the other hand,
is based on the analytic result of Ref. [12].

8 Summary

In this work we have examined, for the first time, the effects of light quark masses on bottom quark
mass determinations based on sum rules for the $\Upsilon$ mesons at NNLO in the non-relativistic expansion.
The effects coming from the charm quark mass are of particular interest, because one of the relevant
physical scales governing the dynamics of the bottom–antibottom quark pair described in the sum
rules is the inverse Bohr radius $M_b \alpha_s$, which is as large as the charm quark mass. Thus, a naive
expansion in the charm quark mass is a priori not possible in the calculations for the sum rules and
the extraction of the bottom quark masses. Based on a NNLO analysis our result is that the charm
mass effects amount to a shift of $-20 \text{ MeV}$ in the bottom 1S mass, the mass parameter that is extracted
directly from the sum rules. Our final result for the bottom 1S mass reads

$$
M_b^{1S} = 4.69 \pm 0.03 \text{ GeV},
$$

(170)
where the error arises from renormalization scale variations; the correlation to the value of the strong coupling is negligible. The bottom 1S mass is a short-distance mass, designed to be used in systems where the bottom quark virtuality is small with respect to its mass. Except for non-relativistic bottom–antibottom quark systems, it can also be applied directly to B meson decays. For inclusive semileptonic rates, it leads to very well behaved perturbative expansions [20]. Starting from the result for the bottom 1S mass in Eq. (170), we have examined the light quark mass effects in the determination of the bottom \( \overline{\text{MS}} \) mass. Here, after rounding to 10 MeV precision, we find another shift of \(-10 \text{ MeV}\) coming from the finite charm quark mass. Our final result for the bottom \( \overline{\text{MS}} \) mass reads

\[
\overline{M}_b(\overline{M}_b) = 4.17 \pm 0.05 \text{ GeV},
\]  

(171)

where the 50 MeV error includes the error in \( M^\text{1S}_b \), in the strong coupling \( (\alpha_s^{(5)}(M_Z) = 0.118 \pm 0.003) \), the perturbative error estimated from variations of the renormalization scale \( \mu \) and the uncertainties in the charm mass corrections. Equation (171) represents a determination of the bottom \( \overline{\text{MS}} \) mass at order \( \alpha_3^3 \). A handy approximation formula that shows the dependence of \( \overline{M}_b(\overline{M}_b) \) on the previously mentioned parameters can be found in Eq. (168). We note that the charm quark mass effects in the bottom 1S mass obtained from the sum rule analysis and those obtained in the relation between the bottom \( \overline{\text{MS}} \) and 1S masses have the same sign and lead to an overall shift of about \(-30 \text{ MeV}\) in \( \overline{M}_b(\overline{M}_b) \). We emphasize that, for all practical applications, the values for the bottom 1S and \( \overline{\text{MS}} \) masses should, in contrast to the pole mass, not be considered as order-dependent numbers, since they do not contain an ambiguity of order \( \Lambda_{QCD} \). Therefore, the results shown in Eqs. (170) and (171) can be used as an input for calculations at any order of perturbation theory.

The order of magnitude of the charm mass corrections in the bottom \( \overline{\text{MS}} \) mass can be anticipated from general considerations because the fact that one cannot expand in \( m_{\text{charm}}/(M_b \alpha_s) \) in the bottom 1S–pole mass relation, whereas it is allowed to expand in \( m_{\text{charm}} \) in the bottom pole–\( \overline{\text{MS}} \) mass relation, leads to a non-analytic correction \( \propto \alpha_s^2 m_{\text{charm}} \) that is \( \pi^2 \)-enhanced and governed by the renormalization scale \( m_{\text{charm}} \) rather than \( M_b \). The enhancement of the linear charm mass term can be understood from the fact that terms that are non-analytic in the square of the light quark masses are sensitive to small (infrared) momenta, in analogy to the non-analytic fictitious gluon mass terms that are often used in standard renormalon analyses. We have explicitly checked that the charm quark mass effects are under control in the bottom \( \overline{\text{MS}} \)-1S mass relation, i.e. they do not lead to an uncontrollable higher order uncertainty that would be relevant at present (or in the foreseeable future). This is because at higher orders of perturbation theory the charm quark (with finite mass) effectively decouples. It was one of the main motivations of this work to study the subtle interplay of the two mechanisms just mentioned at NNLO in the non-relativistic expansion.

In this work we have determined the complete light quark mass corrections for the bottom 1S mass obtained from the \( \Upsilon \) sum rules at NNLO in the non-relativistic expansion, and for the bottom \( \overline{\text{MS}} \) at order \( \alpha_3^3 \), with the following exceptions: in the moments for the sum rules, we neglected the NNLO double-insertion corrections from the NLO static potential at second order Rayleigh–Schrödinger perturbation theory, since they are suppressed with respect to the single-insertion contributions coming from the NNLO static potential at first order Rayleigh–Schrödinger perturbation theory. For the charm mass corrections in the bottom pole–\( \overline{\text{MS}} \) mass relation we have only taken into account the linear charm quark mass terms \( \propto m_{\text{charm}} \) and have neglected higher order terms \( (m_{\text{charm}}/M_b)^n m_{\text{charm}} \) for \( n \geq 1 \). This is feasible because the bottom pole–\( \overline{\text{MS}} \) mass relation does not involve the inverse
Bohr radius as a dynamical scale and because the subleading terms are less sensitive to small momenta and, therefore, not enhanced. We demonstrated that the linear charm mass approximation deviates from the full result for the charm mass corrections by only 10% for the cases where the full result is known. Finally, we have neglected the order $\alpha_s^2$ light quark mass corrections $\propto \alpha_s^2(m_{\text{charm}}/M_b)^n$ for $n \geq 2$ in the short-distance Wilson coefficient of the NRQCD bottom quark currents that describe bottom–antibottom production and annihilation in the non-relativistic regime. The neglected terms are small because the short-distance coefficient only contains contributions from momenta of order $M_b$, which means that an expansion in the charm quark mass is justified. We estimate that all charm mass corrections that have been neglected in this work are an order of magnitude smaller than the ones that have been taken into account. We estimate the effects of the neglected terms and the uncertainties coming from the error in value of the charm quark mass to be at most at the level of 5 MeV.

*Note added:* After this paper was completed we received Ref. [60], where the N$^3$LO large-$\beta_0$ corrections in the heavy quark pole–1S mass relation where presented. The results agree with ours in App. B.

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**A NNLO Light Quark Mass Corrections to the S-Wave Heavy Quark–Antiquark Ground State Mass**

In this appendix we present details of the calculation of the light quark mass corrections to the ground state mass of the heavy-quark–antiquark $J^{PC} = 1^{--}, \, 3S_1$ bound state at NNLO in the non-relativistic expansion. The result is presented using the pole mass definition for the heavy and the light quark masses. We assume that the dynamics of the heavy-quark–antiquark pair is perturbative, i.e. that the scales $M_Q$, $M_Q v$ and $M_Q v^2$ are assumed to be larger than $\Lambda_{QCD}$. We also assume that there are $n_l$ light quarks, of which one quark species has a finite pole mass $m$. We adopt the definition of the strong coupling where all $n_l$ light quarks species contribute to the running.

The formal expressions for the light quark mass corrections up to NNLO have been presented in Eqs. (61) and (62). In configuration space representation the expressions shown in Eqs. (61) and (62) read ($x = |x|, \, y = |y|$):

$$-2 M_Q \Delta_{\text{massive}}^{\text{NLO}} = \int d^3 x \phi_{1S} (x) \delta V_{\text{c.m.}}^{\text{NLO}} (x) \phi_{1S} (x),$$  \hspace{1cm} (172)
\[-2M^\text{pole}}_Q \Delta^{\text{NNLO}}_{\text{massive}} = \int d^3x \phi_{1S}(x) \delta V_{c,m}^{\text{NNLO}}(x) \phi_{1S}(x) - \int d^3x \int d^3y \phi_{1S}(x) \delta V_{c,m}^{\text{NNLO}}(x) \bar{G}_{1S}(x,y) \delta V_{c,m}^{\text{NNLO}}(y) \phi_{1S}(y) - 2 \int d^3x \int d^3y \phi_{1S}(x) \delta V_{c,m}^{\text{NNLO}}(x) \bar{G}_{1S}(x,y) V_{1S}^{\text{NNLO}}(c,massless) \phi_{1S}(y), \quad (173)\]

where \(V_{c,massless}^{\text{NNLO}}(r), \delta V_{c,m}^{\text{NNLO}}(r), \text{and } \delta V_{c,m}^{\text{NNLO}}(r) \) are given in Eqs. (3), (18) and (30), respectively. The term \(\phi_{1S} \) is the LO ground state wave function (see Eq. (179)) and

\[
\bar{G}_{1S}(x,y) = \sum_{\text{S-wave, } i \neq 1} \langle x| i \rangle \langle i | y \rangle \]

is the S-wave component of the configuration space LO Coulomb Green function \(G_c(x,y,E) \) for \(E = E_{1S} = -2M^\text{pole}_Q \Delta^{\text{LO}}_Q \), where the ground state \(n = 1, ^3S_1 \) energy-pole is subtracted. For the calculation of the NNLO light quark mass corrections only the sum over intermediate S-wave states has to be considered, because the light quark mass corrections to the static potential are spin- and angle-independent. An explicit expression for \(\bar{G}_{1S}(x,y) \) can be easily derived from the S-wave \((l = 0)\) contribution of the configuration space Coulomb Green function representation by Voloshin \[55\] \((a_s \equiv a_s^{(n)}(\mu), M \equiv M^\text{pole}_Q)\),

\[
G_{c}^{l=0}(x,y,E) = \frac{M}{4\pi} \frac{2k}{e^{-k(x+y)}} \sum_{n=1}^{\infty} \frac{L_{n-1}^1(2k x) L_{n-1}^1(2k y)}{(n - \frac{3}{2}) n}, \quad (175)\]

where

\[
\gamma = \frac{M^\text{pole}_Q C_F a_s}{2}, \quad (176)\]

\[
k^2 = -M E, \quad (177)\]

and \(L_n^a \) are the generalized Laguerre polynomials. The result reads

\[
\bar{G}_{nS}(x,y) = \lim_{E \rightarrow E_{nS}} \left[ G_{c}^{l=0}(x,y,E) - \frac{\phi_{nS}(x)\phi_{nS}(y)}{E_{nS} - E} \right] = \frac{M \gamma}{2\pi n} \exp\left(-\frac{\gamma}{n}(x+y)\right) \left\{ -\frac{2\gamma}{n^2} \left[ x L_{n-2}^2(\frac{2\gamma}{n} x) L_{n-1}^1(\frac{2\gamma}{n} y) + y L_{n-1}^1(\frac{2\gamma}{n} x) L_{n-2}^2(\frac{2\gamma}{n} y) \right] \right.
\]

\[
+ \left( \frac{5}{2n^2} - \frac{\gamma}{n^3}(x+y) \right) L_{n-1}^1(\frac{2\gamma}{n} x) L_{n-1}^1(\frac{2\gamma}{n} y) \right.
\]

\[
+ \left. \sum_{m \neq n} \frac{L_{m-1}^1(\frac{2\gamma}{n} x) L_{m-1}^1(\frac{2\gamma}{n} y)}{(m-n)m} \right\}, \quad (178)\]

for the subtraction of the \(n \, ^3S_1 \) energy pole, where

\[
\phi_{nS}(x) = \pi^{-1/2} n^{-5/2} \gamma^\frac{n}{2} \exp\left(-\frac{\gamma}{n} x\right) L_{n-1}^1(\frac{2\gamma}{n} x), \quad (179)\]

\[
E_{nS} = -\frac{MC_F^2 a_s^2}{4n^2}. \quad (180)\]
For \( n = 1 \) the first term in the curly brackets vanishes because \( L_{-1}^2(x) = 0 \).

In the following we present a number of intermediate results that lead to Eqs. (63) and (64). All results are eventually expressed in terms of the function \( h_i \ (i = 0, \ldots, 7) \), which have been defined in Eqs. (66)–(74).

**Light Quark Mass Corrections at NLO**

The light quark mass corrections at NLO have been determined before in Ref. [61]. They consist of a single insertion of \( \delta V_{\text{NLO}}^{c,m} \) (Eq. (18)) in first order Rayleigh–Schrödinger perturbation theory:

\[
\int d^3r \phi_{1S}^2(r) \delta V_{\text{NLO}}^{c,m}(r) = - \frac{C_F^2 a_s^2}{2} M_{\text{pole}}^2 \left( \frac{a_s}{3 \pi} \right) \left[ \int_1^\infty dx \frac{f(x)}{1 + \frac{m}{2 \pi} x^2} + \ln \left( \frac{m}{2 \pi} \right) + \frac{11}{6} \right]
\]

where

\[
a = \frac{m}{\gamma}.
\]

The function \( h_0 \) can be easily calculated analytically, see Eq. (66).

**Light Quark Mass Corrections at NNLO – Single Insertions**

For the light quark mass corrections at NNLO let us first consider the contributions coming from the single insertion of the NNLO potential at first order Rayleigh–Schrödinger perturbation theory, the first term on the RHS of Eq. (173). We already mentioned in the text after Eq. (30) that the light quark mass corrections to the NNLO static potential can be divided into three different parts, of which each vanishes individually for \( m \rightarrow 0 \). In the following we present the results from these three contributions separately in terms of the functions \( h_i \): \( \tilde{m} = e^{\gamma_E} m, \tilde{\mu} = e^{\gamma_E} \mu \),

\[
\int d^3r \phi_{1S}^2(r) \left( - \frac{C_F a_s}{r} \right) \left[ - \frac{3}{2} \int_1^\infty dx f(x) e^{-2mrx} \left( \beta_0 \left( \ln \left( \frac{4m^2 x^2}{\mu^2} \right) - \text{Ei}(2m x r) - \text{Ei}(-2m x r) \right) - a_1 \right) 
\right.
\]

\[
+ 3 \left( \ln(\tilde{m} r) + \frac{5}{6} \right) \left( \beta_0 \ln(\tilde{\mu} r) + \frac{a_1}{2} \right) + \beta_0 \frac{\pi^2}{4} \right] \]

\[
= - \frac{C_F^2 a_s^2}{2} M_{\text{pole}}^2 \left[ - \frac{3}{2} h_0(a) \left( \beta_0 \ln \left( \frac{4 \gamma_E^2}{\mu^2} \right) - a_1 \right) - 3 \beta_0 h_1(a) 
\right.
\]

\[
+ 3 \left( \ln \left( \frac{a_2}{2} \right) + \frac{11}{6} \right) \left( \beta_0 \ln \left( \frac{\mu^2}{2 \gamma_E^2} \right) + \beta_0 + \frac{a_1}{2} \right) + \frac{3}{4} \beta_0 (\pi^2 - 4) \right],
\]

\[
\int d^3r \phi_{1S}^2(r) \left( \frac{C_F a_s}{r} \right) \left[ \int_1^\infty dx f(x) e^{-2mrx} \left( \frac{5}{3} + \frac{1}{2x^2} \left( 1 + \frac{1}{2x} \sqrt{x^2 - 1} (1 + 2x^2) \ln \left( \frac{x - \sqrt{x^2 - 1}}{x + \sqrt{x^2 - 1}} \right) \right) 
\right.
\]

\[
+ \int_1^\infty dx f(x) e^{-2mrx} \left( \ln(4x^2) - \text{Ei}(2m x r) - \text{Ei}(-2m x r) - \frac{5}{3} \right) \left. \right]
\]

59
\[ + \left( \ln(\tilde{m} r) + \frac{5}{6} \right)^2 + \frac{\pi^2}{12} \]

\[ = - \frac{C_F^2 a_s^2}{2} M_{Q}^{\text{pole}} \left\{ - h_2(a) + h_0(a) \left( 2 \ln \left( \frac{a}{2} \right) + \frac{5}{6} \right) - 2 h_1(a) + \left( \ln \left( \frac{a}{2} \right) + \frac{11}{6} \right)^2 + \frac{\pi^2}{4} - 1 \right\}, \]  

(184)

\[ \int d^3 r \phi_{1S}^2(r) \left( - \frac{C_F a_s}{r} \right) \left[ \frac{57}{4} \left( c_1 \Gamma(0, 2 c_2 m r) + d_1 \Gamma(0, 2 d_2 m r) + \ln(\tilde{m} r) + \frac{161}{228} + \frac{13}{19} \zeta_3 \right) \right] \]

\[ = - \frac{C_F^2 a_s^2}{2} M_{Q}^{\text{pole}} \left[ \frac{57}{4} \left( c_1 c_2 a - \frac{d_1 d_2 a}{1 + d_2 a} + c_1 \ln(1 + c_2 a) + d_1 \ln(1 + d_2 a) \right) \right]. \]  

(185)

**Light Quark Mass Corrections at NNLO – Double Insertions**

For the light quark mass corrections at NNLO coming from double insertions of the NLO static potential at second order Rayleigh–Schrödinger perturbation theory, there are two different contributions: the first contains two insertions of the NLO light quark mass corrections to the static potential, and the second contains one insertion of the NLO light quark mass corrections to the static potential and one insertion of the NLO static potential for massless light quarks. In detail, the two contributions read:

\[ - \int d^3 x \int d^3 y \phi_{1S}(x) \delta V_{c_m}^{\text{NNLO}}(x) G_{1S}(x, y) \delta V_{c_m}^{\text{NNLO}}(y) \phi_{1S}(y) \]

\[ = \frac{C_F^2 a_s^2}{2} M_{Q}^{\text{pole}} \left\{ h_0(a) \left( - \frac{5}{2} h_0(a) + 2 h_3(a) - 2 h_4(a) \right) - h_5(a) + h_6(a) \right. \]

\[ - 3 h_0(a) \left( \ln \left( \frac{a}{2} \right) + \frac{3}{2} \right) + 2 h_7(a) + 2 h_3(a) \left( \ln \left( \frac{a}{2} \right) + \frac{11}{6} \right) \]

\[ - \frac{1}{2} \ln^2 \left( \frac{a}{2} \right) - \frac{5}{6} \ln \left( \frac{a}{2} \right) - \zeta_3 + \frac{\pi^2}{6} - \frac{61}{72} \right\}. \]  

(186)

\[ - 2 \int d^3 x \int d^3 y \phi_{1S}(x) \delta V_{c_m}^{\text{NNLO}}(x) G_{1S}(x, y) V_{c,massless}^{\text{NNLO}}(y) \phi_{1S}(y) \]

\[ = \frac{C_F^2 a_s^2}{2} M_{Q}^{\text{pole}} \left\{ \frac{3}{2} \beta_0 \left( h_0(a) \left( 3 \ln \left( \frac{2 \gamma}{\mu} \right) - 2 \right) + 2 h_7(a) + 2 h_3(a) \left( 1 - \ln \left( \frac{2 \gamma}{\mu} \right) \right) \right) \right. \]

\[ \left. + \left( \ln \left( \frac{a}{2} \right) + \frac{5}{6} \right) \ln \left( \frac{2 \gamma}{\mu} \right) - 2 \zeta_3 + \frac{\pi^2}{3} - 1 \right) \]

\[ + \frac{3}{2} a_1 \left( - \frac{3}{2} h_0(a) + h_3(a) - \frac{1}{2} \ln \left( \frac{a}{2} \right) - \frac{5}{12} \right) \right\}. \]  

(187)

Adding the two results we arrive at the expression displayed in Eq. (80).
In this appendix we calculate the mass of the ground state of the heavy-quark–antiquark system at $N^3\text{LO}$ in the non-relativistic expansion (or order $\epsilon^4$ in the upsilon expansion) in the large-$\beta_0$ approximation, in terms of the heavy quark pole mass. It is assumed that the dynamics of the heavy quark pair is perturbative, i.e. that $M_Q \gg M_Q \alpha_s \gg M_Q \alpha_s^2 \gg \Lambda_{\text{QCD}}$. All light quarks are treated as massless.

Up to NNLO in the non-relativistic expansion, the large-$\beta_0$ corrections can be easily extracted from the corrections shown in Eq. (53) (for zero light quark masses) by taking the highest power of $n_l$ and supplementing the result by the replacement $n_l \rightarrow -\frac{3}{2} \beta_0$.

Up to $N^3\text{LO}$ the heavy-quark–antiquark ground state mass in the large-$\beta_0$ approximation can be parametrized in the following way:

$$
\left[ M_{Q\bar{Q}}^{n=1} \right]_{\beta_0} = 2M_{Q\bar{Q}}^{\text{LO}} \left[ 1 - \epsilon \Delta_{\beta_0}^{\text{LO}} - \epsilon \Delta_{\beta_0}^{\text{NLO}} - \epsilon \Delta_{\beta_0}^{\text{NNLO}} - \epsilon \Delta_{\beta_0}^{\text{NNNLO}} \right],
$$

(188)

where $(a_s = \alpha_s^{(n_l)}(\mu))$

$$
\Delta_{\beta_0}^{\text{LO}} = \frac{C_F}{8} a_s^2,
$$

(189)

$$
\Delta_{\beta_0}^{\text{NLO}} = \frac{C_F}{8} a_s^2 \left( \frac{a_s}{\pi} \right) \beta_0 \left[ L + \frac{11}{6} \right],
$$

(190)

$$
\Delta_{\beta_0}^{\text{NNLO}} = \frac{C_F}{8} a_s^2 \left( \frac{a_s}{\pi} \right)^2 \beta_0^2 \left[ \frac{3}{4} L^2 + \frac{9}{4} L + \frac{1}{2} \zeta_3 + \frac{\pi^2}{24} + \frac{77}{48} \right],
$$

(191)

$$
L = \ln \left( \frac{\mu}{C_F a_s M_{Q\bar{Q}}^{\text{pole}}} \right).
$$

(192)

To calculate $\Delta_{\beta_0}^{\text{NNNLO}}$ we first need the $N^3\text{LO}$ heavy-quark–antiquark static potential in the large-$\beta_0$ approximation. In momentum space representation the large-$\beta_0$ corrections are particularly simple because they only involve insertions of massless quark one-loop vacuum polarizations into the gluon line defining the LO static potential, supplemented by the replacement $n_l \rightarrow -\frac{3}{2} \beta_0$,

$$
\tilde{V}_{\beta_0}(p) = -\frac{4\pi C_F a_s}{p^2} \left\{ 1 - \left( \frac{a_s}{4\pi} \right) \beta_0 \left[ \ln \left( \frac{p^2}{\mu^2} \right) - \frac{5}{3} \right] + \left( \frac{a_s}{4\pi} \right)^2 \beta_0^2 \left[ \ln \left( \frac{p^2}{\mu^2} \right) - \frac{5}{3} \right]^2 \\
- \left( \frac{a_s}{4\pi} \right)^3 \beta_0^3 \left[ \ln \left( \frac{p^2}{\mu^2} \right) - \frac{5}{3} \right]^3 + \ldots \right\}.
$$

(193)

In configuration space representation, the large-$\beta_0$ potential reads

$$
V_{\beta_0}(r) = \int \frac{d^3p}{(2\pi)^3} \tilde{V}_{\beta_0}(p) \exp(ipr)
= V_{\beta_0}^{\text{LO}}(r) + V_{\beta_0}^{\text{NLO}}(r) + V_{\beta_0}^{\text{NNLO}}(r) + V_{\beta_0}^{\text{NNNLO}}(r) + \ldots,
$$

(194)
where \( \tilde{\mu} \equiv e^{i\pi} \mu \), \( r = |r| \)

\[
V_{\text{LO}}(r) = -\frac{C_F a_s}{r},
\]

\[
V_{\beta_0}^{\text{NNLO}}(r) = -\frac{C_F a_s}{r} \left( \frac{a_s}{2\pi} \right) \beta_0 \left[ \ln(\tilde{\mu} r) + \frac{5}{6} \right],
\]

\[
V_{\beta_0}^{\text{NNNLO}}(r) = -\frac{C_F a_s}{r} \left( \frac{a_s}{2\pi} \right)^2 \beta_0^2 \left[ \left( \ln(\tilde{\mu} r) + \frac{5}{6} \right)^2 + \frac{\pi^2}{12} \right],
\]

\[
V_{\beta_0}^{\text{NNNLO}}(r) = -\frac{C_F a_s}{r} \left( \frac{a_s}{2\pi} \right)^3 \beta_0^3 \left[ \left( \ln(\tilde{\mu} r) + \frac{5}{6} \right)^3 + \frac{\pi^2}{4} \left( \ln(\tilde{\mu} r) + \frac{5}{6} \right) + 2 \zeta_3 \right].
\]

It is now straightforward to derive the formal result for \( \Delta_{\beta_0}^{\text{NNNLO}} \) using Rayleigh–Schrödinger time-independent perturbation theory up to third order:

\[
-2 M_{Q}^{\text{pole}} \Delta_{\beta_0}^{\text{NNNLO}} = \langle 1S | V_{\beta_0}^{\text{NNNLO}} | 1S \rangle + 2 \sum \sum \langle 1S | V_{\beta_0}^{\text{NNLO}} | 1S \rangle \frac{\langle i | \langle i | V_{\beta_0}^{\text{NLO}} + 2 M_{Q}^{\text{pole}} \Delta_{\beta_0}^{\text{NLO}} \rangle | n \rangle | n \rangle | V_{\beta_0}^{\text{NLO}} | 1S \rangle,
\]

\[
= \int d^3 x \phi_{1S}(x) V_{\beta_0}^{\text{NNNLO}}(x) \phi_{1S}(x)
- 2 \int d^3 x \int d^3 y \phi_{1S}(x) V_{\beta_0}^{\text{NLO}}(x) G_{1S}(x,y) V_{\beta_0}^{\text{NLO}}(y) \phi_{1S}(y)
+ \int d^3 x \int d^3 y \int d^3 z \phi_{1S}(x) V_{\beta_0}^{\text{NLO}}(x) G_{1S}(x,y) \left( V_{\beta_0}^{\text{NLO}}(y) + 2 M_{Q}^{\text{pole}} \Delta_{\beta_0}^{\text{NLO}} \right)
\times G_{1S}(y,z) V_{\beta_0}^{\text{NLO}}(z) \phi_{1S}(z),
\]

where

\[
\phi_{1S}(r) = \langle r | 1S \rangle = \langle 1S | r \rangle = \pi^{-\frac{3}{2}} \gamma^{\frac{3}{2}} e^{-\gamma r},
\]

\[
\gamma = \frac{M_{Q}^{\text{pole}} C_F a_s}{2},
\]

is the LO ground state Coulomb wave function and \( G_{1S}(x,y) \) the S-wave component of the Coulomb Green function, where the ground state energy pole is subtracted. The explicit form of \( G \) is given in Eq. (178). The reader should note the appearance of the NLO binding energy in the third term on the RHS of Eq. (199), which arises for the first time at third order Rayleigh–Schrödinger perturbation theory (see e.g. Ref. [62]). For the calculation of the integrals in Eq. (199) the following formulae are helpful (\( a_c \equiv C_F \alpha_s^{(m)}(\mu) \), \( x = |x|, y = |y|, z = |z| \)):

\[
A_1^0 = \int d^3 x \phi_{1S}^2(x) \left[ -\frac{a_c}{x} \right] = -a_c \gamma,
\]

\[
A_1^1 = \int d^3 x \phi_{1S}^2(x) \left[ -\frac{a_c}{x} \ln(\tilde{\mu} x) \right] = -a_c \gamma \left[ \ln \left( \frac{\mu}{2 \gamma} \right) + 1 \right],
\]

62
\[ A_1^3 = \int d^3 x \, \frac{a_c}{x} \ln^3(\bar{\mu} x) \]
\[ A_2^3 = \int d^3 x \, \frac{a_c}{x} \ln^3(\bar{\mu} x) \]
\[ = - a_c \gamma \left[ \ln^3 \left( \frac{\mu}{2 \gamma} \right) + 3 \ln^2 \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^2}{2} \ln \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^2}{2} - 2 \zeta_3 \right], \quad (205) \]
\[ A_2^1 = - \int d^3 x \, \int d^3 y \, \phi_{1S}(x) \left[ - \frac{a_c}{y} \ln(\bar{\mu} y) \right] \phi_{1S}(y) \]
\[ = - a_c \gamma \left[ \frac{1}{2} \ln \left( \frac{\mu}{2 \gamma} \right) \right], \quad (206) \]
\[ A_2^2 = - \int d^3 x \, \int d^3 y \, \phi_{1S}(x) \left[ - \frac{a_c}{x} \ln(\bar{\mu} x) \right] \tilde{G}_{1S}(x, y) \phi_{1S}(y) \]
\[ = - a_c \gamma \left[ \ln^3 \left( \frac{\mu}{2 \gamma} \right) + 3 \ln^2 \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^2}{2} \ln \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^2}{2} + 4 \zeta_3 - 1 \right], \quad (207) \]
\[ A_3^3 = \int d^3 x \, \int d^3 y \, \int d^3 z \, \phi_{1S}(x) \left[ - \frac{a_c}{z} \ln(\bar{\mu} z) \right] \tilde{G}_{1S}(x, y) \tilde{G}_{1S}(y, z) \left[ - \frac{a_c}{z} \ln(\bar{\mu} z) \right] \phi_{1S}(z) \]
\[ = - \frac{1}{2} \left[ \frac{3}{2} \ln^2 \left( \frac{\mu}{2 \gamma} \right) + \frac{1}{2} \ln \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^4}{45} - \frac{2 \pi^2}{3} + \frac{9}{2} \right], \quad (209) \]
\[ A_3^3 = \int d^3 x \, \int d^3 y \, \int d^3 z \, \phi_{1S}(x) \left[ - \frac{a_c}{x} \ln(\bar{\mu} x) \right] \tilde{G}_{1S}(x, y) \left[ - \frac{a_c}{y} \ln(\bar{\mu} y) \right] \tilde{G}_{1S}(y, z) \left[ - \frac{a_c}{z} \ln(\bar{\mu} z) \right] \phi_{1S}(z) \]
\[ = - a_c \gamma \left[ \frac{3}{4} \ln^3 \left( \frac{\mu}{2 \gamma} \right) + \frac{\pi^4}{90} - \frac{\pi^2}{3} + \frac{5}{2} \right] \ln \left( \frac{\mu}{2 \gamma} \right) \]
\[ + \frac{\pi^4}{40} - \frac{\pi^2}{6} + 6 \zeta_5 - \left( \frac{\pi^2}{2} + 4 \right) \zeta_3 + \frac{15}{4} \zeta_5 \zeta_3, \quad (210) \]

Using Eqs. (202)–(210) it is straightforward to derive the result for \( \Delta_{\beta_0}^{NNNLO} \):

\[ \Delta_{\beta_0}^{NNNLO} = \frac{C_F}{8} \left( \frac{a_s}{\pi} \right)^3 \beta_0^3 \left[ \frac{1}{2} L^3 + \frac{15}{8} L^2 + \left( \frac{\pi^2}{12} + \zeta_3 + \frac{25}{12} \right) L \right. \]
\[ + \frac{\pi^4}{1440} + \frac{19 \pi^2}{144} + 2 \zeta_5 - \left( \frac{\pi^2}{8} - \frac{11}{6} \right) \zeta_3 + \frac{517}{64} \zeta_3 \zeta_5 \zeta_3 + \frac{517}{64}, \quad (211) \]
where
\[
L = \ln \left( \frac{\mu}{2\gamma} \right).
\]  

(212)

C  Order \( \alpha_s^4 \) \( \overline{\text{MS}}-1S \) Mass Relation in the Large-\( \beta_0 \) Approximation

In this appendix we determine the order \( \alpha_s^4 \) (or order \( \epsilon^4 \) in the upsilon expansion) relation between the heavy quark \( \overline{\text{MS}} \) and 1S masses in the large-\( \beta_0 \) approximation. We assume that there are \( n_l \) light quarks that are all massless.

The large-\( \beta_0 \) approximation of the heavy quark \( \overline{\text{MS}} \)-pole mass relation is known to all orders of perturbation theory. The all order formula based on the resummation of massless quark one-loop vacuum polarization insertions into the one-loop gluon line reads \[41\] (\( \bar{a}_s = \alpha_s^{(n_l)}(M_Q) \))

\[
\left[ \frac{M_Q(M_Q) - M_Q^{\text{pole}}}{M_Q^{\text{pole}}} \right]_{\beta_0} = -\sum_{n=0}^{\infty} \bar{a}_s \left[ \left( \frac{\bar{a}_s}{4\pi} \right)^2 \beta_0 \right]^n \left( \frac{d}{du} \right)^n \left\{ \frac{1}{3\pi} \left( \frac{e^{\frac{3}{2}u} 6(1-u)}{G(u) G(1-2u)} + \frac{\tilde{B}(u)}{u} \right) \right\} \bigg|_{u=0},
\]  

(213)

where

\[
\tilde{B}(u) = \sum_{n=0}^{\infty} \frac{u^n}{(n!)^2} \left( \frac{d}{du} \right)^n B(u) \bigg|_{u=0},
\]  

(214)

\[
B(u) = -\frac{1}{3} (3+2u) \frac{\Gamma(4+2u)}{\Gamma(1-u) \Gamma(2+u) \Gamma(3+u)}.
\]  

(215)

We note that in the large-\( \beta_0 \) approximation the actual definition of the heavy quark mass as the renormalization scale in Eq. (213) is irrelevant, because this only affects subleading corrections in the large-\( \beta_0 \) approximation. Evaluating Eq. (213) up to order \( \alpha_s^4 \) we arrive at

\[
\left[ \frac{M_Q(M_Q)}{M_Q^{\text{pole}}} \right]_{\beta_0} = M_Q^{\text{pole}} \left[ 1 - \epsilon \delta^{(1)} - \epsilon^2 \delta^{(2)}_{\beta_0} - \epsilon^3 \delta^{(3)}_{\beta_0} - \epsilon^4 \delta^{(4)}_{\beta_0} - \ldots \right],
\]  

(216)

where

\[
\delta^{(1)} = \frac{4}{3} \left( \frac{\bar{a}_s}{\pi} \right),
\]  

(217)

\[
\delta^{(2)}_{\beta_0} = \left( \frac{\bar{a}_s}{\pi} \right)^2 \beta_0 \left( \frac{\pi^2}{12} + \frac{71}{96} \right),
\]  

(218)

\[
\delta^{(3)}_{\beta_0} = \left( \frac{\bar{a}_s}{\pi} \right)^3 \beta_0^2 \left( \frac{7}{24} \zeta_3 + \frac{13\pi^2}{144} + \frac{2353}{10368} \right),
\]  

(219)

\[
\delta^{(4)}_{\beta_0} = \left( \frac{\bar{a}_s}{\pi} \right)^4 \beta_0^3 \left( \frac{71\pi^4}{7680} + \frac{317}{468} \zeta_3 + \frac{89\pi^2}{1152} + \frac{42979}{331776} \right).
\]  

(220)
The large-$\beta_0$ approximation for the $\overline{\text{MS}}$–1S mass relation up to order $\alpha_s^4$ ($\epsilon^4$) using the upsilon expansion (with $\epsilon = 1$) then reads
\[
\left[ \overline{M}_Q(M_Q) \right]_{\beta_0} = M_Q^{1S} \left[ 1 + \epsilon \left( \Delta^{\text{LO}} - \delta^{(1)} \right) + \epsilon^2 \left( \Delta^{\text{NLO}} - \delta^{(2)} \right) \right. \\
+ \epsilon^3 \left( \Delta^{\text{NNLO}} - \delta^{(3)} \right) + \epsilon^4 \left( \Delta^{\text{NNNLO}} - \delta^{(4)} \right) + \cdots, \quad (221)
\]
where the $\Delta$’s are given in Eqs. (189)–(191) and (211). We note that, in contrast to the complete result, the inversion of Eq. (188) is particularly simple in the large-$\beta_0$ approximation because higher powers of low order contributions can be dropped. This is because they do not contain the highest power of $n_l$ in any order of perturbation theory.

D Three-Loop Light Quark Mass Corrections to the Heavy Quark Pole–$\overline{\text{MS}}$ Mass Relation from Vacuum Polarization Insertions

In this appendix we present analytic results for the functions $f_P^{(0)}$, $f_P^{(1)}$ and $f_{PP}^{(0)}$ (see Sec. 3), which occur in the order $\alpha_s^2$ and $\alpha_s^3$ corrections in the relation between the heavy quark $\overline{\text{MS}}$ and the pole mass, and which come from insertions of massive quark one-loop vacuum polarizations into the gluon line ($r \equiv m/M_Q$):
\[
f_P^{(0)} \left( \frac{m}{M_Q} \right) = \frac{1}{4} \int_0^\infty dq^2 \left[ \frac{1}{2} \frac{q^2}{M_Q^2} + \left( 1 - \frac{1}{2} \frac{q^2}{M_Q^2} \right) \left( 1 + 4 \frac{M_Q^2}{q^2} \right) \frac{1}{2} \right] P \left( \frac{m^2}{q^2} \right)
\]
\[
= \frac{3}{2} \ln^2(r) + \frac{\pi^2}{4} - \frac{3}{2} \left( \ln(r) + \frac{3}{2} \right) r^2 \\
+ \frac{3}{2} \left( 1 + r \right) \left( 1 + r^2 \right) \left( \text{Li}_2(-r) - \frac{1}{2} \ln(r)^2 - \ln(r) \ln(1 + r) + \frac{\pi^2}{6} \right) \\
+ \frac{3}{2} \left( 1 - r \right) \left( 1 - r^2 \right) \left( \text{Li}_2(r) - \frac{1}{2} \ln(r)^2 + \ln(r) \ln(1 - r) - \frac{\pi^2}{3} \right), \quad (222)
\]
\[
f_P^{(1)} \left( \frac{m}{M_Q} \right) = \frac{1}{4} \int_0^\infty dq^2 \left[ \frac{1}{2} \frac{q^2}{M_Q^2} + \left( 1 - \frac{1}{2} \frac{q^2}{M_Q^2} \right) \left( 1 + 4 \frac{M_Q^2}{q^2} \right) \frac{1}{2} \right] P \left( \frac{m^2}{q^2} \right) \ln \left( \frac{q^2}{M_Q^2} \right)
\]
\[
= \frac{3}{4} r^2 \left( \frac{1}{2} - \ln(r) \right) + r^4 \ln^2(r) \left( \frac{3}{4} - \ln(r) \right) - \frac{1}{2} (1 - 5 r - 5 r^3 + r^4) \ln^2(1 + r)
\]
\[
- \frac{\pi^2}{4} \left( \frac{r}{4} (6 - 4 r + 6 r^2 - r^3) - r (5 + 5 r^2 + r^3) \ln(r) + (1 + 7 r + 7 r^3 + r^4) \ln(1 + r) \right)
\]
\[
- \frac{3}{4} (1 + r)^2 (1 + r^2) \left( \ln(1 - r^2) \ln(r) + \frac{1}{2} \text{Li}_2(r^2) \right)
\]
\[
- 3 r (1 + r^2) \left( - \frac{7 \pi^2}{6} \ln(2) + \frac{1}{3} \ln^3(2) - \ln(1 - r) \ln(r) (1 - 2 \ln(2r)) \\
+ \ln(2) \ln(1 + r) \ln \left( \frac{1 + r}{2} \right) - 2 \ln(r) \ln(1 + r) \ln \left( \frac{2 r (1 - r)}{1 + r} \right) \right)
\]
65
The function $P$ has been defined in Eq. (15). The result for $f_1$ is new.

The results for $f_2$ are new.

The function $P$ has been defined in Eq. (15). The result for $f_{PP}^{(0)}$ has already been obtained in Ref. [34]. The results for $f_{PP}^{(1)}$ and $f_{PP}^{(0)}$ are new.

\[
f_{PP}^{(0)} \left( \frac{m}{M_Q} \right) = \frac{1}{4} \int_0^\infty dq^2 \left[ \frac{1}{2} \frac{q^2}{M_Q^2} + \left( 1 - \frac{1}{2} \frac{q^2}{M_Q^2} \right) \left( 1 + 4 \left( \frac{M_Q^2}{q^2} \right)^2 \right) \right] \left[ P \left( \frac{m^2}{q^2} \right) \right]^2
\]

\[
= \frac{4}{5} (1 - r^2) r^2 + \frac{3}{2} (6 - 7 r - 7 r^3) \zeta_3 - \frac{4}{5} (1 + 2 r^2) r^2 \ln(r)
\]

\[
+ \frac{\pi^2}{30} r (96 - 30 r + 120 r^2 - 65 r^3 + 8 r^5) + \pi^2 (1 + 7 r + 7 r^3 + r^4) \ln(1 + r)
\]

\[- \frac{1}{5} r (1 - r) (32 + 17 r + 57 r^2 - 8 r^3 - 8 r^4) \ln(1 - r) \ln(r)
\]

\[+ \frac{1}{5} r (1 + r) (32 - 17 r + 57 r^2 + 8 r^3 - 8 r^4) \ln(1 + r) \ln(r)
\]

\[- \frac{1}{5} r^2 (30 + 65 r^2 - 8 r^4) \ln^2(r) + 6 (1 + r)^2 (1 - r^2) \ln(1 - r) \ln^2(r)
\]

\[+ (1 - 5 r - 5 r^3 + r^4) \ln^3(1 + r) + \frac{8}{5} r (4 + 5 r^2) \left( \Li_2(-r) - \Li_2(r) \right)
\]

\[+ \left( 3 \left( 2 + 3 r^4 \right) \ln(r) + \frac{1}{10} r^2 (15 + 65 r^2 - 8 r^4) \right) \Li_2(r^2) - 3 (1 + 2 r^4) \Li_3(r^2)
\]

\[+ 6 r (1 + r^2) \left( - \frac{\pi^2}{6} (7 \ln(2) + 2 \ln(r)) + \frac{1}{3} \ln^3(2)
\]

\[+ \ln \left( \frac{1 + r}{2} \right) \left( 2 \ln(r) \ln \left( \frac{1 + r}{1 - r} \right) + \ln(2) \ln(1 + r) \right) + 2 \ln(r) \Li_2 \left( \frac{1 - r}{1 + r} \right)
\]

\[+ 2 \Li_3 \left( \frac{1}{1 + r} \right) + 2 \Li_3 \left( \frac{2 r}{1 + r} \right) - 2 \Li_3 \left( \frac{1 + r}{2} \right)
\]

\[+ 6 (1 - r^2) (1 + r^2) \left( \ln(1 + r) \ln^2(r) - \Li_3(1 - r)
\]

\[- \Li_3 \left( \frac{1}{1 + r} \right) + \frac{1}{2} \Li_3(1 - r^2) \right).
\]

The function $P$ has been defined in Eq. (15). The result for $f_{P}^{(0)}$ has already been obtained in Ref. [34]. The results for $f_{P}^{(1)}$ and $f_{PP}^{(0)}$ are new.
Some Formulae for Moments with Massless Light Quarks

In this appendix the expressions for the constants \( w_0^0, w_1^1, w_2^2 \) are given. They have been taken from Ref. [7]. They arise in the charm quark mass corrections to the moments of the \( \Upsilon \) sum rules if the charm quark is included in the evolution of the strong coupling. The constants read \((p = 1, 2, 3, \ldots)\):

\[
\begin{align*}
\frac{w_0^0}{p! \Gamma\left(\frac{p}{2}\right)} = & - \frac{1}{\Gamma\left(\frac{p}{2}\right)} \int_0^\infty \int_0^\infty \frac{1}{(1 + t + u)^2} \ln^p \left(\frac{(1 + t)(1 + u)}{t u}\right) = - \frac{(p + 1) \zeta_{p+1}}{\Gamma\left(\frac{p}{2}\right)}, \\
\frac{w_1^1}{p! \Gamma\left(\frac{p}{2}\right)} = & \frac{1}{\Gamma\left(\frac{p}{2}\right)} \int_0^\infty \int_0^\infty \frac{1 - \ln(1 + t + u)}{(1 + t + u)^2} \ln^p \left(\frac{(1 + t)(1 + u)}{t u}\right) \\
& = - \left\{ \frac{(1 + p)}{\Gamma\left(\frac{p}{2}\right)} \left[ \gamma_E \zeta_{p+1} + \sum_{m=0}^\infty \frac{\Psi(2 + m)}{(1 + m)^{p+1}} \right] + \frac{2}{\Gamma\left(\frac{p}{2}\right)} \sum_{l=0}^{p-1} \sum_{m=0}^\infty (-1)^{p-l} \frac{(1 + l) \Psi(p-l)(2 + m)}{(p-l)!(1 + m)^{l+1}} \right\}, \tag{225}
\end{align*}
\]

\[
\begin{align*}
\frac{w_2^2}{p! \Gamma\left(\frac{p}{2}\right)} = & \frac{1}{\Gamma\left(\frac{p}{2}\right)} \int_0^\infty \int_0^\infty \frac{\zeta_2 - 2 \ln(1 + t + u) + \ln^2(1 + t + u)}{(1 + t + u)^2} \ln^p \left(\frac{(1 + t)(1 + u)}{t u}\right) \\
& = \frac{(1 + p)}{\Gamma\left(\frac{p}{2}\right)} \left\{ (\gamma_E^2 + 2 \zeta_2) \zeta_{1+p} \\
& + \sum_{m=0}^\infty \frac{1}{(1 + m)^{1+p}} \left[ 2 \gamma_E \Psi(2 + m) - \Psi'(2 + m) + \left(\Psi(2 + m)\right)^2 \right] \right\} \\
& + \frac{2}{\Gamma\left(\frac{p}{2}\right)} \sum_{m=0}^\infty \sum_{l=0}^{p-1} \frac{(-1)^{p-l} (1 + l)}{(p-l)!(1 + m)^{l+1}} \left[ 2 \gamma_E \Psi(p-l)(2 + m) - \Psi(p-l+1)(2 + m) \\
& + 2 \Psi(p-l)(2 + m) \Psi(2 + m) \right] \\
& + \frac{4}{\Gamma\left(\frac{p}{2}\right)} \sum_{m=0}^\infty \sum_{l=0}^{p-2} \sum_{k=1}^{p-l-1} \frac{(-1)^{p-l} (1 + l) \Psi(p-l-k)(2 + m) \Psi(k)(2 + m)}{(p-l-k)!(1 + m)^{l+1}} \right\}. \tag{226}
\end{align*}
\]

References


