High-precision $\alpha_s$ determination from bottomonium sum rules

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The strong coupling, $\alpha_s$, governs perturbative Quantum Chromodynamics (QCD) and is one of the free parameters of the Standard Model. We introduce a new method for determining $\alpha_s(m_Z)$ with high precision from dimensionless ratios of roots of moments of the bottom-quark vector correlator. The ratios we use in our analysis have a rather weak logarithmic quark-mass dependence, starting at $O(\alpha_s^2)$, and can be obtained from experimental data with high precision, since they benefit from positive correlations among the individual experimentally determined moments. We perform a careful and conservative error analysis with special emphasis on uncertainties related to the truncation of perturbation theory, treating the renormalization scales such as to ensure order-by-order convergence. Our final result, with expressions at $O(\alpha_s^3)$, is $\alpha_s(m_Z) = 0.1186 \pm 0.0015$, one of the most precise extractions of the QCD coupling from experimental data to date.

Significant progress has been made in the past few years to extract $\alpha_s$ with good precision, which requires effort both in experimental measurements or lattice simulations, as well as in theoretical computations, in order to reach higher levels of accuracy which depend, in particular, on calculations at higher loop order. Extractions based on lattice data, especially, have improved considerably in the recent past. However, several tensions still remain, what has led the Particle Data Group to enlarge the uncertainty on its recommended $\alpha_s(m_Z)$ world average\textsuperscript{2} by about $\sim 50\%$ with respect to the 2016\textsuperscript{3} edition. It remains, therefore, very important to find reliable observables to extract the strong coupling, in which both theory and experiment are under very good control. In this paper we describe for the first time the use of ratios of roots of moments of the bottom-quark vector correlator in precise extractions of $\alpha_s$.

One of the standard observables in QCD is the total cross section for $e^+e^- \rightarrow$ hadrons and the associated $R_{q\bar{q}}(s)$ ratio defined as

$$ R_{q\bar{q}}(s) = \frac{3s}{4\pi\alpha^2} \sigma_{e^+e^- \rightarrow q\bar{q} + X}(s) \approx \frac{\sigma_{e^+e^- \rightarrow q\bar{q} + X}(s)}{\sigma_{e^+e^- \rightarrow \mu^+\mu^-}(s)} \quad (1) $$

where $\alpha$ is the fine-structure constant, $\sqrt{s}$ is the $e^+e^-$ center-of-mass energy, and the right-hand side is exact when the denominator is calculated in the limit of massless muons and at leading order in $\alpha$. Integrated moments of $R_{q\bar{q}}(s)$ play a prominent role, since they make use of data in broad energy regions, as opposed to considering the observable locally, which can significantly improve their experimental precision and the reliability of their theoretical description. These integrated moments can also be, in many cases, rigorously calculated in perturbation theory. In this work, the inverse moments of $R_{b\bar{b}}(s)$ defined as

$$ M_{b}^{(n)} = \int_{s_0}^{\infty} \frac{ds}{s^{n+1}} R_{b\bar{b}}(s) \quad (2) $$

are specially important, where $s_0$ must be smaller than the squared mass of the first $b\bar{b}$ narrow resonance, the $\Upsilon(1S)$. They have been, so far, mainly used in the precise extraction of the $c$- and $b$-quark masses from data. In the present work, for reasons that will become clear soon, we are interested in dimensionless ratios of roots of moments $M_{b}^{(n)}$

$$ R_{b}^{V,n} \equiv \left( \frac{M_{b}^{(n)}}{M_{b}^{(n+1)}} \right)^{\frac{1}{n+1}} \quad (3) $$

where $V$ refers to the fact that the moments are related to the vector bottom-quark current correlator. Analogous ratios of moments have originally been introduced in the context of the pseudo-scalar charm correlator for which only lattice data is available\textsuperscript{4}. As we will show, the ratios $R_{b}^{V,n}$ that we introduce here are particularly suitable for $\alpha_s$ extractions: for $1 \leq n \leq 3$ they are known up


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to $\mathcal{O}(\alpha_s^3)$, have a very weak dependence on the $b$-quark mass, and can be accurately determined using the experimental values for the masses and partial widths of narrow resonances, supplemented with continuous data for $R_{b\bar{b}}(s)$.

Let us start by discussing the perturbative expansion for $M_b^{(n)}$ and the ratios $R_b^{V,n}$. Using analyticity and unitarity, the moments $M_b^{(n)}$ can be related to derivatives of the vector-bottom-quark current correlator. The theoretical counterpart to Eq. (2) reads

$$M_b^{(n)} = \frac{12\pi^2 Q_q^2}{n!} \frac{\alpha_s(\mu)}{\pi} \left( \frac{\mu}{m_b} \right)^n \begin{bmatrix} \alpha_s(\mu) \end{bmatrix}^i,$$

where $Q_q$ is the quark electric charge and the correlator is formed from the quark currents as

$$(g^{\mu\nu} s - p^\mu p^\nu) \Pi_b(s) = -i \int dx e^{i p \cdot x} \langle 0 | T j_b^\mu(x) j_b^\nu(0) | 0 \rangle,$$  

with $j_b^\mu(x) = \bar{b}(x) \gamma^\mu b(x)$. The Taylor coefficients of the $\Pi_b(s)$ expansion in powers of $s$ around $s = 0$, that participate in Eq. (4), can be accurately calculated in perturbation theory with the typical short-distance scale given by $\sim m_b/n > \Lambda_{\text{QCD}}$ (restricting $n$ to small values). In full generality, the perturbative expansion of $M_b^{(n)}$ is written in terms of two renormalization scales, $\mu_s$, at which the strong coupling is evaluated, and $\mu_m$, where the quark-mass is evaluated:

$$M_b^{(n)} = \frac{1}{2 m_b(\mu_m)^2} \sum_{i=0}^{[i-1]} \bigg[ \sum_{a=0}^{[i-1]} c_i^{(n)}(\mu_f) \ln^a \left( \frac{\mu_f}{m_b(\mu_f)} \right) \ln^b \left( \frac{\mu_f}{m_b(\mu_f)} \right) \bigg].$$

The leading logarithm in $M_b^{(n)}$ appears at order $\alpha_s$. Setting the two scales in Eq. (6) to the common value $\mu_f = \mu_m = m_b(\bar{m}_b)$ the logarithms are resummed and the expansion of $M_b^{(n)}$ in this particular case exposes the independent coefficients $c_i^{(n)}$, which must be calculated in perturbation theory. Thanks to a tremendous computational effort, the coefficients $c_i^{(n)}$ have been calculated (analytically) for $n = 1, 2, 3$ and 4 \cite{10} up to order $\alpha_s^3$ [four loops, or next-to-next-to-next-to-leading order (N$^3$LO)]. For $n > 4$ only estimates are available at this order. The logarithms of Eq. (6) with the respective coefficients can be generated with the use of renormalization group equations. Numerical values of the coefficients $c_i^{(n)}$ can be found in Ref. 13. The dependence of $M_b^{(n)}$ on $m_b$ through the prefactor makes these moments ideal for the extraction of the bottom-quark mass.

The ratios we are interested in, given in Eq. (3), are constructed in such a way as to cancel the mass dependence of the prefactor in Eq. (4). Their fixed-order perturbative expansion reads

$$R_b^{V,n} = \sum_{i=0}^{[i-1]} \sum_{j=0}^{[i-1]} \sum_{k=0}^{[i-1]} r_i^{(n)}(\mu_m) \ln^j \left( \frac{\mu_m}{m_b(\mu_m)} \right) \ln^k \left( \frac{\mu_m}{m_b(\mu_m)} \right),$$

where now the first logarithm, which brings the dependence on $m_b$, appears only at $\alpha_s^2$. The ratios $R_b^{V,n}$ are, therefore, almost insensitive to the quark mass. The coefficients $r_i^{(n)}(\mu_m)$ can be obtained from $c_i^{(n)}(\mu_m)$ upon renormalization group equations. For instance, for $R_b^{V,2}$ at N$^3$LO one finds

$$R_b^{V,2} = 0.82937 + 0.47645 a_s + (0.24518 + 1.8264 L_\alpha) a_s^2 - (2.8544 + 3.6528 L_m - 4.1826 L_\alpha - 7.0012 L_m^2) a_s^3,$$

with $\alpha_s = \alpha_s(\mu_f)/\pi$, $L_\alpha = \ln[\alpha_s(\mu_f)/m_b(\mu_m)]$, and $L_m = \ln[m_f/m_b(\mu_m)]$. The leading $\alpha_s$ correction to $R_b^{V,1}$ is of about 4.5%, for $R_b^{V,2}$ it is 2.2%, and for $R_b^{V,3}$ it is 1.4%. The perturbative contribution to $R_b^{V,n}$ is the first term in its Operator Product Expansion (corresponding to the identity operator). The leading non-perturbative correction stems from the gluon condensate and is known to $\mathcal{O}(\alpha_s)$ \cite{14}. In the case of bottom-quark moments, this correction is tiny and hence taken into account only as check that non-perturbative effects are fully under control. We have included it into our analysis, but the effect is completely immaterial and will no longer be discussed here. Our results are, therefore, overwhelmingly dominated by perturbative QCD.

We turn now to the experimental determination of the ratios $R_b^{V,n}$. Our results are based on the obtention of the inverse moments $M_b^{(n)}$ performed in Ref. 13 and discussed in detail in that work. One must combine the contribution from the first four narrow resonances with the threshold data from BABAR \cite{15}. The latter has to be corrected for initial-state radiation and vacuum polarization effects. An unfolding of the data is necessary, which introduces correlations among the different data points. This results in moments $M_b^{(n)}$ with strong correlations. BABAR data are available only up to 11.2 GeV. The remainder contribution to the integral of Eq. (2) is modeled with perturbation theory for $R_{s\bar{s}}(s)$, often referred to as the continuum contribution. Moments with higher values of $n$ are, by construction, less sensitive to how the continuum is treated. In the case of quark-mass
extractions, one normally fixes the input value of $\alpha_s$ in the continuum. Here, however, since we aim at extracting $\alpha_s$ from data, one cannot do this lest the results be contaminated by the input value of the strong coupling. We have, therefore, adapted the extraction of the moments $M_b^{(n)}$ from Ref. [13] in order to obtain $R_b^{V,n}$ as a function of the $\alpha_s$ value used in the continuum. It turns out that the dependence with $\alpha_s$, for values not too far from the world average, is highly linear, which facilitates the task of obtaining parametrized expressions for the ratios $R_b^{V,n}$. In terms of $\Delta_\alpha = 0.1181 - \alpha_s$, the three ratios we exploit here read

$$
R_b^{V,1} = (0.8020 + 0.4083 \Delta_\alpha) \pm 0.0014,
$$
$$
R_b^{V,2} = (0.84647 + 0.14955 \Delta_\alpha) \pm 0.00040,
$$
$$
R_b^{V,3} = (0.89617 + 0.06905 \Delta_\alpha) \pm 0.00017.
$$

The associated errors are completely dominated by data and are very small. The smallness of the errors is in part due to the strong positive correlations between the consecutive moments $M_b^{(n)}$ which, when properly propagated, lead to a very small uncertainty in the ratios. (For example, moments $M_b^{(2)}$ and $M_b^{(3)}$ are 86% correlated.) The relative errors in the ratios are of only 0.16%, 0.046%, 0.019% for $R_b^{V,1}$, $R_b^{V,2}$, and $R_b^{V,3}$, respectively.

The determination of $\alpha_s$ is done by equating the experimental results of $R_{b,s}$ to the respective expansions of the type of Eq. (8), numerically solving for $\alpha_s$. We turn now to a discussion of the results we obtain from this analysis. Sound results require a careful and conservative study of the associated uncertainties, in particular those that stem from the truncation of the perturbative series. It has been shown that in quark-mass extractions from $M_b^{(n)}$, a reliable error estimate requires the independent variation of the two scales $\mu_m$ and $\mu_\alpha$ [13]. To be fully conservative, even though here the dependence on $\mu_m$ is weaker than in the case of $M_b^{(n)}$, we vary both scales in the interval $\mu_b = \mu_\alpha, \mu_m = \mu_{max}$, with $\mu_{max} = 15$ GeV, and apply the constraint $1/\xi \leq (\mu_\alpha/\mu_m) \leq \xi$ with the canonical choice $\xi = 2$ (the dependence on the value of $\xi$ will be discussed below). The scale variation we adopt is much more conservative than that used in many related works, where one often sets $\mu_m = \mu_\alpha$ (or $\xi = 1$). For the bottom mass we adopt the current world average $\mu_b = 4.180(23)$ GeV. With this setup we have created grids with 4000 points of $\mu_{max}$ and $\mu_\alpha$ and the respective $\alpha_s$ values for each ratio $R_b^{V,n}$ (with $n = 1, 2, 3$), order by order in the perturbative expansion. First, we check the convergence of the $\alpha_s$ extractions at each order in perturbation theory from the results obtained in the grids, without considering any other source of uncertainty apart from the spread in values due to scale variation, which measures the perturbative error. The results are shown in Fig. 2 for the three ratios we consider. One clearly sees a nice convergence for all the moments, which indicates that the perturbative uncertainties are under control.

We continue the investigation of perturbative uncertainties by analyzing the $\alpha_s$ grids with two-dimensional contour plots at NLO. In Fig. 3 we show the result of such a scan in the case of $R_b^{V,2}$. What one sees from this plot is that a correlated scale variation with $\mu_\alpha = \mu_m$, along the diagonal of the plot, would lead to a seriously underestimated theory uncertainty. The consequences of a correlated scale variation would be less dramatic for $n = 1$ and $n = 3$ but the results of Fig. 2 demonstrate, visually, the need of the independent scale variation. Fi-

\[\text{Fig. 2. Results for } \alpha_s \text{ from } R_b^{V,2} \text{ at } O(\alpha_s^2) \text{ in the } \mu_\alpha \times \mu_m \text{ plane. Shaded areas are excluded from our analysis (see text).}\]
nally, to examine systematically the consequences of less (and more) conservative scale variations, we vary the value of $\xi$ between $\xi = 1$, which corresponds to $\mu_\alpha = \mu_n$, and $\xi = 3$, that imposes no constraint. For $\xi = 1$ we find that the perturbative uncertainties would be underestimated by 46% to 136% (depending on the ratio) compared to our canonical choice ($\xi = 2$). Adopting even more conservative choices, on the other hand, would lead to increases in the errors by at most 40%, which shows that our canonical choice is sufficient for a conservative error estimate. The central values of $\alpha_s$ are, on the other hand, rather stable with the choice of $\xi$ and the variations are below the percent level for $1 \leq \xi \leq 3$.

With the perturbative uncertainties under good control, we are in a position to extract the final values of our analysis. To study the other sources of uncertainties we created additional $\alpha_s$ grids in the $\mu_n \times \mu_\alpha$ plane varying within one sigma the experimental value of $R_b^{V,n}$ and the bottom-quark mass. We find, through the analysis of these grids,

\[
\alpha_s(m_Z) = 0.1183(11)^{\text{pert}}(25)^{\text{exp}} = 0.1183(28)^{\text{tot}}[R_b^{V,1}],
\alpha_s(m_Z) = 0.1186(12)^{\text{pert}}(09)^{\text{exp}} = 0.1186(15)^{\text{tot}}[R_b^{V,2}],
\alpha_s(m_Z) = 0.1194(14)^{\text{pert}}(05)^{\text{exp}} = 0.1194(14)^{\text{tot}}[R_b^{V,3}],
\]

where the first error is due to the truncation of perturbation theory, obtained from the the spread of values arising from the independent scale variation, and the second comes from the experimental errors given in Eq. (9).

The total error is obtained adding the first two in quadrature. In all cases the uncertainty associated with the bottom-quark mass is $\leq 0.0002$ and does not contribute to the final error. Likewise, the error associated with non-perturbative effects, estimated through the gluon condensate contribution, is completely insignificant given the scale of the overall error (as previously mentioned).

The final results for $\alpha_s$ are correlated since they are based on ratios of moments obtained from the same data sets. This disfavors averaging the results obtained from the different ratios $R_b^{V,n}$. Instead, we quote as our final value the one obtained from the ratio $R_b^{V,2}$. The reasons for this choice are the following. The experimental uncertainty, in the case of the extraction from $R_b^{V,1}$, is significantly larger which makes the final error much less competitive. The extraction from $R_b^{V,3}$, on the other hand, relies on $M_0^{(4)}$ which may have a too large value of $n$ and correspondingly a smaller effective scale — a fact that may be responsible for the somewhat larger perturbative uncertainty. The most reliable result is therefore the one from $R_b^{V,2}$ which yields our final value

\[
\alpha_s^{(n=5)}(m_Z) = 0.1186 \pm 0.0015. \tag{10}
\]

Our result is fully compatible with the present world average $[0.1181(11)]$ [22] and has a comparable uncertainty. Our determination has a very conservative error estimate: with a correlated scale variation the uncertainty would be reduced to 0.0010, below the world average’s. Comparison with other works in the literature show that our perturbative error is also more conservative than what is obtained from estimates of higher-order contributions (as opposed to scale variations). Our treatment of the experimental moments is also completely unbiased, since we do not fix $\alpha_s$ to compute the continuum contribution, but keep it as a free parameter: freezing the value of $\alpha_s$ in the experimental moments would essentially keep the central value unchanged, but our final uncertainty would be 0.0011, which again attests the conservative character of our analysis. Our result is compared with other selected recent extractions of $\alpha_s$ in Fig. 3.

The present analysis can be extended in a number of directions. First, it can directly be applied to the vector moments of the charm-quark current. Preliminary results show that the errors on $\alpha_s$ in this case are not as competitive as the ones from the bottom. One can also apply our more conservative treatment of perturbative uncertainties to analyze pseudo-scalar current moments obtained on the lattice. Our results on these additional analyses will be presented elsewhere, together with further details on the results from the bottom-quark current. On the theory side, one could also investigate alternative ways of organizing the perturbative expansion, such as using different powers of $R_b^{V,n}$ (re-expanded in $\alpha_s$) or linearized iterative solutions (in the spirit of [13]). Additionally, the cancellation of the renormalon associated with the pole mass when taking ratios allows for an analysis that employs directly the pole mass in the log-

![FIG. 3. Comparison of our determination of $\alpha_s^{(n=5)}(m_Z)$ (top, in red) with a few recent determinations. Event-shape analyses at N3LL + $O(\alpha_s^3)$; thrust and C-parameter (green) [16,17]; lattice QCD [4,19,22] and static energy potential [23] (in dark blue); Electroweak precision observables fits [24] (black); Deep Inelastic Scattering [25] and global PDF fits [26,27] (light blue); and hadronic $\tau$ decays [28,29] (gray). The current world average [3] is shown as an orange band.](image-url)
arithms. One could also consider fits using all available information (including correlations) in order to extract $\alpha_s$ and the quark-masses in a self-consistent way. We plan to carry out these analyses in the future.

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