Precision Determination of Heavy Quark Masses and the Strong Coupling Constant

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We present a new QCD sum rule with high sensitivity to the continuum regions of charm and bottom quark pair production. Combining this sum rule with existing ones yields very stable results for the $\overline{\rm MS}$ quark masses, $\hat{m}_c(\hat{m}_c)$ and $\hat{m}_b(\hat{m}_b)$. We introduce a phenomenological parametrization of the continuum interpolating smoothly between the pseudoscalar threshold and asymptotic quark regions. Comparison of our approach with recent BES data allows for a robust theoretical error estimate. The parametric uncertainty due to α_s is reduced by performing a simultaneous fit to the most precise sum rules and other high precision observables. This includes a new evaluation of the lifetime of the τ lepton, τ_τ, serving as a strong constraint on α_s. Our results are $\hat{m}_c(\hat{m}_c) = 1.289^{+0.040}_{-0.045}$ GeV, $\hat{m}_b(\hat{m}_b) = 4.207^{+0.030}_{-0.031}$ GeV (with a correlation of 29%), and $\alpha_s(M_Z)[\tau_\tau] = 0.1221^{+0.0026}_{-0.0023}$.

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The determination of the fundamental Standard Model (SM) parameters is important not only in its own right, but also as a SM test when results from various sources are compared. Such comparisons can foster our understanding of SM dynamics (such as strong QCD effects) or may ultimately lead to hints of new physics beyond the SM. Moreover, precise values of the SM parameters can be compared against the predictions of more fundamental theories. Well known examples are Grand Unified Theories [1] which typically predict values for the strong coupling constant, α_s, and the mass ratio m_b/m_τ.

It is generally difficult to obtain reliable information on quark masses. The Particle Data Group [2] lists only ranges for their values, indicating a lack of confidence in the theoretical methods used to evaluate them. Indeed, α_s is quite large at the mass scales of the bottom and charm quarks, questioning the convergence of perturbative QCD (PQCD). Furthermore, non-perturbative (power suppressed) effects governed by the scale $\Lambda_{\rm QCD} \sim 0.5$ GeV could be large, thus compromising reliable calculations. Two types of conditions are known to improve the situation: high energy or inclusiveness. As an example for the former, α_s and m_b can be determined at LEP energies using PQCD. This yields $\alpha_s(M_Z) = 0.1200 \pm 0.0028$ [3] with very little theoretical uncertainty, but b quark effects are small and $\hat{m}_b(M_Z) = 2.67 \pm 0.50$ GeV [4] is not well constrained.

In this Letter, we compute α_s from τ_τ, by definition an inclusive quantity and known to be quite insensitive to effects from non-perturbative QCD (NPQCD) [5]. Likewise, we use a set of inclusive QCD sum rules to derive values for $\hat{m}_c(\hat{m}_c)$ and $\hat{m}_b(\hat{m}_b)$. One of these sum rules is new, and its use together with existing ones [6, 7] proves to be a powerful tool to constrain the continuum region of quark pair production. This will be particularly helpful for the case of the b quark for which precise measurements of $R(s)$ (the inclusive hadronic cross section normalized to the leptonic point cross section) or of $R_b(s)$ (exclusive cross section for $b\bar{b}$ pairs) are unavailable.

On the basis of an unsubtracted dispersion relation (UDR) it was shown in Ref. [8] that knowledge of m_c, m_b, and α_s is sufficient to compute the charm and bottom quark contributions to the QED coupling $\alpha(\sqrt{t} = M_Z)$, a vital parameter entering the analysis of the very high precision LEP 1 and SLC data. Or conversely, comparison of this UDR with the more traditional approach using a subtracted dispersion relation (SDR) offers information on m_c and m_b. The resulting equation relates an inclusive integrated cross section to a difference of vacuum polarization tensors, *viz.*

$$12\pi^2 \left[\hat{\Pi}_q(0) - \hat{\Pi}_q(-t)\right] = t \int_{4m_q^2}^{\infty} \frac{{\rm d}s}{s} \frac{R_q(s)}{s+t}. \qquad (1)$$

Eq. (1) defines a continuous set of sum rules parametrized by t, where the limit $t \to 0$ coincides with the first moment of $\Pi_q(t)$. Similarly, there is a sum rule,

$$\frac{12\pi^2}{n!} \frac{d^n}{dt^n} \Pi_q(t)\bigg|_{t=0} = \int_{4m_q^2}^{\infty} \frac{{\rm d}s}{s^{n+1}} R_q(s), \qquad (2)$$

for each higher moment, $\mathcal{M}_n$, as well [6, 7, 9, 10, 11]. We now take the opposite limit in Eq. (1), $t \to \infty$, and regularize the divergent expression (which will render $\mathcal{M}_0 < 0$!),

$$\frac{R_q(s)}{3Q_q^2} \longrightarrow \frac{R_q(s)}{3Q_q^2} - \lambda_1^q(s) \equiv \frac{R_q(s)}{3Q_q^2} - 1 - \frac{\alpha_s(\sqrt{s})}{\pi} - \left[\frac{\alpha_s(\sqrt{s})}{\pi}\right]^2 \left[\frac{365}{24} - 11\zeta(3) + n_q\left(\frac{2}{3}\zeta(3) - \frac{11}{12}\right)\right]. \qquad (3)$$

Q_q and n_q are the quark charge and the number of active flavors. Using expressions derived in Refs. [12, 13], we can now explicitly write down the sum rule (1) for $t \to \infty$:

$$\sum_{\text{resonances}} \frac{3\pi\Gamma_R^e}{Q_q^2 M_R \hat{\alpha}^2(M_R)} + \int_{4M^2}^{\infty} \frac{ds}{s} \frac{R_q^{\rm cont}}{3Q_q^2} - \int_{\hat{m}_q^2}^{\infty} \frac{ds}{s} \lambda_1^q(s)$$

$$= -\frac{5}{3} + \frac{\hat{\alpha}_s}{\pi}\left[4\zeta(3) - \frac{7}{2}\right] + \frac{\hat{\alpha}_s^2}{\pi^2}\left[\frac{11}{4}\zeta(2) + \frac{2429}{48}\zeta(3) - \frac{25}{3}\zeta(5) - \frac{2543}{48} + n_q\left(\frac{677}{216} - \frac{\zeta(2)}{6} - \frac{19}{9}\zeta(3)\right)\right]. \quad (4)$$

Here, M_R and Γ_R^e are the mass and the electronic partial width of resonance R, and $R_q^{\rm cont}$ denote the continuum regions integrated from $M = M_{B^\pm}$ for b and $M = M_{D^0}$ for c. The $\zeta(2)$ terms arose from the regularization (3) which together with the scale choices $\hat{m}_q = \hat{m}_q(\hat{m}_q)$ and $\hat{\alpha}_s = \hat{\alpha}_s(\hat{m}_q)$ eliminates (resums) all logarithmic terms in Eq. (4). Unlike in any of the sum rules (2), $R_q^{\rm cont}$ appears unsuppressed in Eq. (4) so that $\hat{m}_q$ varies exponentially with the experimental information on the resonances. An optimal approach to compute $\alpha(M_Z)$ would first identify the sum rule most sensitive to m_q, and then use the value so obtained in theoretical expressions such as the one presented in Ref. [8]. We will use Eq. (4) to constrain the continuum region and work with the following *ansatz*:

$$\frac{R_q^{\rm cont}(s)}{3Q_q^2} = \lambda_1^q(s)\sqrt{1 - \frac{4\,\hat{m}_q^2(2M)}{s'}}\left[1 + \lambda_3^q \frac{2\,\hat{m}_q^2(2M)}{s'}\right] \approx$$

$$\lambda_1^q(4M^2)\sqrt{1 - \frac{4\,\hat{m}_q^2}{s'}}\left[1 + \lambda_3^q \frac{2\,\hat{m}_q^2}{s'}\right] - \frac{\hat{\alpha}_s}{\pi}\frac{\lambda_2^q(s)}{1 + \lambda_2^q(s)}, \quad (5)$$

where now $\hat{\alpha}_s = \hat{\alpha}_s(2M)$, $s' \equiv s + 4(\hat{m}_q^2(2M) - M^2)$, and

$$\lambda_2^q(s) = \frac{\hat{\alpha}_s}{\pi}\beta_0 \ln\frac{s}{4M^2} = \frac{\hat{\alpha}_s(2M)}{\pi}\left(\frac{11}{4} - \frac{n_q}{6}\right)\ln\frac{s}{4M^2}.$$

We will use the form in the second line (applying it to all moments) of Eq. (5) with the corresponding change in the regularization in Eq. (4). This keeps only the leading logarithms resummed but allows for an analytical integration. Eq. (5) coincides asymptotically with the predictions of PQCD for massless quarks and interpolates smoothly between the vanishing phase space at the pseudoscalar threshold and the strong onset of fermion pair production. The quark parton model predicts $\lambda_3^q = 1$, while from third order massive QCD corrections [14] one expects $\lambda_3^q > 1$ (in agreement with our results). But unlike when PQCD is applied to $R(s)$ directly and relatively close to the resonance region, we minimize the exposure to local quark-hadron duality violations by using QCD *inclusively* and by merely requiring stable results across the moments. No claim is being made about the *local shape* of R_q — we only need theoretical information about *global averages*.

We use the narrow resonance data [2] listed in Table I as the only experimental input. The wider resonances in the continuum region are assumed to be accounted for by our *ansatz* (5) because (i) they decay almost exclusively into flavored hadrons; (ii) they interfere with the non-resonating part of the continuum rendering a common treatment virtually impossible; (iii) the δ-function approximation (which is perfect for the narrow resonances) becomes successively worse; (iv) the philosophy of our *ansatz* supposes that it averages over local cross-section fluctuations; and (v) we wish to compare Eq. (5) directly to experimental data on the charm continuum region such as from Beijing [15]. The narrow resonance contribution

R	M_R [GeV]	Γ_R^e [keV]	R	M_R [GeV]	Γ_R^e [keV]
J/Ψ	3.09687	5.26 (37)	$\Upsilon(1S)$	9.46030	1.320 (50)
$\Psi(2S)$	3.68596	2.19 (15)	$\Upsilon(2S)$	10.02326	0.520 (32)
			$\Upsilon(3S)$	10.35520	0.476 (78)

TABLE I: Resonance data [2] used in the analysis. The uncertainties from the resonance masses are negligible.

n	resonances	continuum	total	theory
0	1.16 (6)	-3.03 ± 0.37	-1.86 ± 0.37	**input** (4)
1	1.12 (6)	1.04 ± 0.14	2.16 ± 0.16	2.19 (6)
2	1.10 (7)	0.37 ± 0.07	1.47 ± 0.10	1.49 (9)
3	1.10 (7)	0.17 ± 0.04	1.27 ± 0.08	1.26 (14)
4	1.11 (7)	0.09 ± 0.02	1.20 ± 0.08	1.16 (20)
5	1.13 (7)	0.05 ± 0.01	1.18 ± 0.08	1.10 (31)
0	1.17 (5)	-52.44 ± 1.24	-51.27 ± 1.24	**input** (2)
1	1.24 (5)	3.12 ± 0.53	4.36 ± 0.54	4.51 (2)
2	1.31 (5)	1.33 ± 0.30	2.64 ± 0.31	2.79 (3)
3	1.40 (5)	0.75 ± 0.19	2.15 ± 0.20	2.27 (5)
4	1.50 (5)	0.48 ± 0.13	1.98 ± 0.14	2.06 (7)
5	1.61 (5)	0.33 ± 0.10	1.94 ± 0.11	1.99 (10)
6	1.74 (6)	0.23 ± 0.07	1.98 ± 0.09	1.98 (14)
7	1.89 (6)	0.17 ± 0.05	2.06 ± 0.08	2.03 (19)

TABLE II: Results for the lowest moments, $\mathcal{M}_n$, defined in Eq. (1) for $n = 0$ ($t \to \infty$) and Eq. (2) for $n \geq 1$. The upper (lower) half of the Table corresponds to the charm (bottom) quark. Each moment has been multiplied by $10^n\,\mathrm{GeV}^{2n}$ ($10^{2n+1}\,\mathrm{GeV}^{2n}$). The continuum error is from $\Delta\lambda_3^{b,c} = \pm 1.47$. The last column shows the theoretical prediction for $\hat{m}_c(\hat{m}_c) = 1.289$ GeV, $\hat{m}_b(\hat{m}_b) = 4.207$ GeV, and $\alpha_s(M_Z) = 0.1211$, where the uncertainty is our estimate for the truncation error (see text).

to the various moments is shown in the second column of Table II. The Γ_R^e are obtained from constrained fits [2] to a great number of measurements independently for each resonance, and should have very small correlations. We will therefore combine their propagated errors in quadrature. The 3rd column gives the continuum contribution, and the 4th column shows the totals to be compared with the theoretical moments in the last column, *viz.*

$$\mathcal{M}_n^{\rm theory} = \frac{9}{4} Q_q^2 \left(\frac{1}{2\hat{m}_q(\hat{m}_q)} \right)^{2n} \bar{C}_n. \qquad (6)$$

The $\bar{C}_n$ are known up to $\mathcal{O}(\alpha_s^2)$ and from Refs. [12, 16] where they were computed for arbitrary renormalization scale μ. It seems appropriate to choose $\mu = \hat{m}_q(\hat{m}_q)$, eliminating all logarithmic terms as there is only one scale in the problem. Indeed, the authors of Ref. [11], who have chosen $\mu = 3$ (10) GeV for the charm (bottom) quark and then evolved to $\mu = \hat{m}_q$, report a variation over the first 5 (7) moments of 122 (312) MeV. (For larger moments the α_s expansion [17] of the gluon condensate contribution [7] breaks down.) Using the same moments [11] but choosing $\mu = \hat{m}_q$ instead, we observe a variation of less than 27 (16) MeV. This impressive improvement clearly overcompensates for the larger $\hat{\alpha}_s$. We will choose $\mu = \hat{m}_q$ in the following. As for the theoretical uncertainty associated with the truncation of the perturbative series, we use the method suggested in Ref. [18]. It exploits the fact that once stripped off all group theoretical factors, the coefficients appearing in PQCD (to the very least for highly inclusive quantities defined in the Euclidean domain) are strictly of order unity[18]. Since one can easily determine the largest group theoretical factor in the next uncalculated perturbative order, this offers a reliable and *transparent* way to assess truncation errors. In our case this yields the error estimate,

$$\pm N_C Q_q^2 C_F C_A^2 \frac{\hat{\alpha}_s^3(\hat{m}_q)}{\pi^3} \left(\frac{1}{2\hat{m}_q(\hat{m}_q)} \right)^{2n}, \qquad (7)$$

($N_C = C_A = 4C_F = 3$) corresponding to $\pm 16\hat{\alpha}_s^3/\pi^3$ in the $\bar{C}_n$. Comparing the corresponding estimate against the exactly known coefficients of the first eight moments up to order α_s^2 [12, 16] shows that with $\mu = \hat{m}_q$, 23 of 24 coefficients are within the estimate, while only one coefficient would have been underestimated by a factor ≈ 1.437. This seems to be a reasonable state of affairs for a 1σ error estimate and corresponds to ± 20 MeV for $\hat{m}_c(\hat{m}_c)$ from $\mathcal{M}_1$, while variation of the renormalization scale [11] assesses this error to only 1 MeV, which is optimistic. We show the estimate (7) in the last column of Table II. The last two columns of that Table would agree within errors even if we had chosen significantly smaller variations in λ_3^b and especially λ_3^c ($\Delta\lambda_3^{b,c} = \pm 1.47$ accounts for the error introduced by our *ansatz* and is above and beyond the variations induced by the fit parameters). The reason for our more conservative error is shown in Table III. It shows that Eq. (5) with $\lambda_3^c = 0.50$ reproduces the n dependence of the moments computed from recent data by the BES Collaboration [15] remarkably well. However, our method favors $\lambda_3^c \approx \lambda_3^b \approx 1.97$, and thus 30 to 40% larger contributions. Table III also compares the BES data to the $\Psi(3S)$ contribution [2] in the narrow width approximation. Even assuming that

n	BES	$\lambda_3^c = 0.50$	$\lambda_3^c = 1.97$	BES	$\Psi(3S)$
0	5.51 (35)	5.50	7.19	0.215 (39)	0.348 (54)
1	3.02 (19)	3.01	3.98	0.151 (27)	0.245 (38)
2	1.68 (11)	1.68	2.25	0.106 (19)	0.172 (27)
3	0.95 (6)	0.96	1.29	0.074 (13)	0.121 (19)
4	0.55 (4)	0.55	0.76	0.052 (9)	0.085 (13)
5	0.32 (2)	0.33	0.45	0.037 (6)	0.060 (9)

TABLE III: The left part shows contributions to the charm moments ($\times 10^{n+1}\text{GeV}^{2n}$) from $2M_{D^0} \leq \sqrt{s} \leq 4.8$ GeV, and the right part from $2M_{D^0} \leq \sqrt{s} \leq 3.83$ GeV. Following Ref. [11], we computed the columns labeled BES by subtracting from the threshold data on $R(s)$ the average, $\bar{R}$, below threshold. (We applied corrections for the leading s-dependence.) The errors combine the statistical and uncorrelated systematic ones of $\bar{R}$ with those in the continuum region and with the common systematics ($\leq 3.5\%$) of the difference.

the $\Psi(3S)$ resonance ($M_{\Psi(3S)} = 3.7699$ GeV) saturates the charm cross-section in that region, we observe a direct *experimental* 2σ discrepancy between Ref. [15] and $\Gamma^e_{\Psi(3S)} = 0.26 \pm 0.04$ keV [2]. Thus there is a discrepency between the theory and the BES data, though the theory does seem to be consistent with the $\Psi(3S)$ data. This constitutes a great puzzle which needs to be resolved in the future. We may be able to quote smaller errors after this situation has been resolved. Nevertheless, the quark masses can still be determined precisely through the sum rule approach.

There is a possible contribution from the gluon condensate [7]. It is known up to $\mathcal{O}(\alpha_s)$ [17], but its actual value is not well known. Its inclusion lowers the extracted quark masses, increases λ_3^c, and sharpens the discrepancy with the BES data. We can bound its value to $\lesssim 0.07$ GeV^4 by demanding n independent results within the uncertainties. We use this bound (with a central value of zero) to account collectively for non-perturbative uncertainties. They induce errors of about 29 MeV into $\hat{m}_c(\hat{m}_c)$ ($n = 2$) and 2.4 MeV into $\hat{m}_b(\hat{m}_b)$ ($n = 6$).

The parametric uncertainties from α_s and the quark masses themselves are correlated in a complicated way (i) across the moments, (ii) across the two quark flavors, (iii) between the theoretical moments and the continuum contribution, and (iv) with each other. In practice, all this is accounted for by performing fits to the moments. Heavy quark radiation by light quarks [19] is not resonating and problems associated with singlet contributions [19, 20] appear only at $\mathcal{O}(\alpha_s^3)$, so these issues should not introduce further uncertainties into our analysis. We will present our final results after discussing the τ lifetime.

For our analysis of the τ mean lifetime,

$$\tau_\tau = \frac{\hbar}{\Gamma_\tau} = \hbar \frac{1 - \mathcal{B}_S}{\Gamma^e_\tau + \Gamma^\mu_\tau + \Gamma^{ud}_\tau} = 290.96 \pm 0.59 \text{ fs}, \qquad (8)$$

we evaluate the partial widths into leptons, $\Gamma^e_\tau + \Gamma^\mu_\tau$, and hadrons with vanishing net strangeness, Γ_τ^{ud}, theoretically. The relative fraction of decays with $\Delta S = -1$, $\mathcal{B}_S = 0.0286 \pm 0.0009$ [2], is based on experimental data, since the value for the strange quark mass, $\hat{m}_s(m_\tau)$, is not well known, and the PQCD expansion, $C_{QCD}^{D=2}$, proportional to m_s^2 converges poorly and cannot be trusted. $C_{QCD}^{D=2}$ also multiplies the corresponding $m_{u,d}^2$ terms in Γ_τ^{ud}, posing the same but numerically less important problem there. We solved it, by relating $C_{QCD}^{D=2}$ to the ratio $\Gamma_\tau^{us}|V_{ud}|^2/(\Gamma_\tau^{ud}|V_{us}|^2) = 0.896 \pm 0.034$ [2] (in which to linear order all universal terms cancel), and find $C_{QCD}^{D=2}(m_s^2 - m_d^2) = m_\tau^2(0.091 \pm 0.046)$. We included one-loop electroweak ($S_{\rm EW}$) [21] and QED (phase space) corrections [22], quark condensate contributions, as well as c quark effects in an expansion in $m_\tau^2/4m_c^2$ [23]. *E.g.*,

$$\Gamma_\tau^{ud} = \frac{G_F^2 m_\tau^5 |V_{ud}|^2}{64\pi^3} S_{\rm EW}(1+\frac{3m_\tau^2}{5M_W^2}) \left[F_{\rm QCD} + \frac{\hat{\alpha}}{\pi}(\frac{85}{24} - \frac{\pi^2}{2}) \right.$$

$$\left. -0.09 \frac{m_u^2 + m_d^2}{m_s^2 - m_d^2} - \frac{f_{\pi^\pm}^2}{m_\tau^4}[m_{\pi^\pm}^2(8\pi^2 + 23\alpha_s^2) - 4m_{K^\pm}^2\alpha_s^2] \right].$$

$F_{\rm QCD} - 1$ is the massless QCD correction. Due to effects governed by the β-function, the 3-loop PQCD expansion [5] shows slow convergence. The series can be reorganized [24] into a well-behaved expansion with coefficients, d_i [14], from the Adler D-function. The new expansion is not a power series. Rather, the d_i multiply complicated functions, $A_i(\alpha_s)$ [24], which we calculate numerically up to 4-loop order in the β function [25].

We computed the world average (8) by combining the direct value, $\tau_\tau = 290.6 \pm 1.1$ fs [2], with $\tau_\tau(\mathcal{B}_e, \mathcal{B}_\mu) = 291.1 \pm 0.7$ fs derived from the leptonic branching ratios $\mathcal{B}_e = 0.1784(6)$ and $\mathcal{B}_\mu = 0.1737(6)$ [2] taking into account their 1% correlation. The dominant theoretical error induced by the unknown coefficient $d_3 = 0 \pm 77$ [18] is itself strongly α_s-dependent, is recalculated in each call within a fit, and induces an asymmetric α_s error.

Other experimental uncertainties arise from [2] $m_\tau = 1.77699(28)$ GeV, $|V_{ud}| = 0.97485(46)$, and $\mathcal{B}_S$. Uncertainties from higher dimensional terms in the operator product expansion, OPE, are taken from Ref. [26] and add up to $\Delta\tau_\tau(\text{OPE}) = \pm 0.64$ fs. We assume that an uncertainty of the same size is induced by possible OPE breaking effects[28]. The unknown five-loop β-function coefficient, $\beta_4 = 0 \pm 579$ [18], contributes mainly to the evolution of $\alpha_s(m_\tau)$ to $\alpha_s(M_Z)$ and less to the A_i. The subleading errors listed in this paragraph amount to ± 1.2 fs. We find, $\alpha_s(m_\tau) = 0.356^{+0.027}_{-0.021}$ and $\alpha_s(M_Z) = 0.1221^{+0.0026}_{-0.0023}$, in excellent agreement with $\alpha_s(M_Z) = 0.1200 \pm 0.0028$ from Z-decays [3] and most other recent evaluations of τ_τ [26, 27]. Including τ_τ, and the $n = 2$ and $n = 6$ moments for the c and b quark, respectively, as constraints in a fit to all data [3] yields,

$$\begin{aligned} \alpha_s(M_Z) &= 0.1211^{+0.0018}_{-0.0017}, \\ \hat{m}_c(\hat{m}_c) &= 1.289^{+0.040}_{-0.045} \text{ GeV}, \\ \hat{m}_b(\hat{m}_b) &= 4.207^{+0.030}_{-0.031} \text{ GeV}. \end{aligned} \tag{9}$$

These results reduce the error [8] in $\alpha(M_Z)$ by 25%.

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[28] It is sometimes speculated that OPE breaking effects could induce dangerous terms of $\mathcal{O}(\Lambda^2_{\mathrm{QCD}}/m^2_\tau)$. The absence of numerically significant terms of that type is difficult to prove with rigor. We stress, however, that the fits to OPE condensate terms of Ref. [26] should have revealed their presence.