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Calculation of the QED Coupling $\hat{\alpha}(M_Z)$ in the Modified Minimal-Subtraction Scheme

Jens Erler
Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104-6396, USA
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I calculate the QED coupling, $\hat{\alpha}$, directly in the $\overline{\rm MS}$ scheme using an unsubtracted dispersion relation for the three light quarks, and perturbative QCD for charm and bottom quarks. Compact analytical expressions are presented, making this approach particularly suitable for electroweak fits. After $\hat{\alpha}^{-1}(m_\tau) = 133.513 \pm 0.026$ is obtained in a first step, I perform a 4-loop renormalization group evolution with 3-loop matching conditions to arrive at $\hat{\alpha}^{-1}(M_Z) = 127.934 \pm 0.027$ for $\hat{\alpha}_s(M_Z) = 0.120$. The corresponding hadronic contribution to the on-shell coupling is $\Delta\bar{\alpha}^{(5)}_{\rm had}(M_Z) = 0.02779 \pm 0.00020$. The error is mainly from m_c, and from experimental uncertainties in e^+e^- annihilation into unflavored and strange hadrons and τ decay data.

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I. INTORDUCTION

The increasing precision of experiments at CERN, SLAC, and the Tevatron calls for refined theoretical calculations with corresponding accuracy. For example, the precision of measurements of M_W, the Z width, and the weak mixing angle, $\hat{s}^2_Z$, has reached or surpassed the per mille level. Most theoretical uncertainties are presently still negligible compared to the experimental ones. In contrast, the QED coupling constant ($\overline{\rm MS}$ quantities will be marked by a caret),

$$\hat{\alpha}(\mu) = \frac{\alpha}{1 - 4\pi\alpha\hat{\Pi}(0)}, \qquad (1)$$

escapes a precise theoretical computation from the fine structure constant, α, for $\mu > 2m_{\pi^0}$ when hadronic effects must be included. On the other hand, knowledge of $\hat{\alpha}(M_Z)$ is indispensable for the extraction of the Higgs mass from precision data. In particular, with m_t known independently from top quark production at the Tevatron, M_W and $\hat{s}^2_Z$ now serve as the most important Higgs probes, but are strongly correlated with $\hat{\alpha}(M_Z)$. Clearly, precise and reliable information on $\hat{\alpha}(M_Z)$ is needed.

This has prompted a great deal of activity in the course of the past 4 years [1–5]. The traditional strategy is to exploit the analytic properties of QCD and obtain a subtracted dispersion relation (SDR) [6] for the on-shell coupling, $\bar{\alpha}(M_Z)$. By virtue of the optical theorem a weighted integral over the e^+e^- cross section ratio,

$$R(s) = 12\pi {\rm Im}\,\hat{\Pi}^{(\rm had)}(s) = \frac{\sigma_{\rm hadrons}}{\sigma_{\mu^+\mu^-}}, \qquad (2)$$

is obtained. The task is now reduced to construct the function $R(s)$ for the entire energy regime $s \geq 4m^2_{\pi^0}$ using both theoretical and experimental information. This is a complex process, and the various papers [1–5] differ by the methods by which experimental data are averaged, by the energy regimes in which perturbative QCD (PQCD) is trusted, by the treatment and parametrization of resonances, etc. The situation is aggravated by the fact that the data sets in question often lack a thorough documentation, and much of the data taking was done at a time when per mille precisions were not anticipated. Consequently, an emancipation from old or imprecise data is indicated whenever possible.

The key question is the energy domain in which the use of PQCD is adequate. PQCD and QCD driven data normalization for energies as low as a few GeV have been advocated by Martin and Zeppenfeld [2], but at the time encountered scepticism. A breakthrough came from three sides. First, theoretical calculations [7] and measurements of the τ lifetime have matured significantly over the last decade, with the extracted strong coupling constant [8], $\hat{\alpha}_s$, in perfect agreement with the value extracted from the Z lineshape [9]. Secondly, in Ref. [8] Höcker studies the invariant mass distribution in τ decays following the spectral moments proposed by Le Diberder and Pich [11]. When varying his input data, he obtains impressively consistent results for the non-perturbative contributions to vector and axial-vector two-point correlation functions, which are moreover fairly small. Having passed this test, Davier and Höcker [3] finally fit to analogously defined spectral moments of $R(s)$, with the conclusion that non-perturbative contributions to $R(m_\tau)$ are negligibly small. Motivated by these developments, Kühn and Steinhauser [4] present a state of the art analysis of the SDR approach.

In this letter I introduce a different method based on an unsubtracted dispersion relation (UDR). This is the natural framework for the computation of $\hat{\alpha}(\mu)$, defined at only one momentum transfer, $q^2 = 0$. By its very concept it is a purely perturbative quantity. Complications from non-perturbative physics arise only to the extent to which dispersion relations are used. This is hard to avoid for the three light flavors, but c and b quarks will turn out to be massive enough to be treated exclusively within PQCD. The approach chosen in this paper also has an important practical advantage. Calculations of Higgs limits or χ^2 plots [9] require thousands of fits each with multiple function calls. A numerical (dispersion) integration within each call would be too expensive computationally, but within the approach introduced in this work, no numerical integration will be necessary. As a result $\hat{\alpha}(M_Z)$ can be self-consistently recalculated in each call, and the parametric uncertainty due to $\hat{\alpha}_s$ (which is a fit parameter) can be dropped.

II. HEAVY QUARKS

The polarization function in Eq. (1) is defined through the current correlator,

$$(q_\mu q_\nu - q^2 g_{\mu\nu})\hat{\Pi}(q^2) = i \int d^4x e^{iqx} \langle 0|T j_\mu(x) j_\nu(0)|0\rangle,$$

where j_μ is the electromagnetic current. For a heavy quark it has been calculated up to 3-loop $\mathcal{O}(\hat{\alpha}\hat{\alpha}_s^2)$ in Ref. [12]. The result for $\hat{\Pi}^{(h)}(0)$ is expressed in terms of the quark pole mass. The coefficients grow rapidly and application to charm (bottom) quarks is impossible (questionable). However, the adverse coefficients are almost entirely due to the employment of the pole mass, which is (due to quark confinement) not a well defined quantity [13]. It is therefore appropriate to reexpress $\hat{\Pi}^{(h)}(0)$ in terms of the $\overline{\rm MS}$ mass, $\hat{m}(\mu)$, yielding (in agreement with Ref. [14]),

$$\hat{\Pi}^{(h)}(0) = \frac{Q_h^2}{4\pi^2}\left\{L + \frac{\hat{\alpha}_s}{\pi}\left[\frac{13}{12} - L\right] + \frac{\hat{\alpha}_s^2}{\pi^2}\left[\frac{655}{144}\zeta(3) - \frac{3847}{864} - \frac{5}{6}L - \frac{11}{8}L^2 + n_q\left(\frac{361}{1296} - \frac{L}{18} + \frac{L^2}{12}\right)\right]\right\}, \quad (3)$$

where Q_h is the electric charge of the heavy quark, n_q the number of active flavors, and $L = \ln\frac{\mu^2}{\hat{m}^2}$. Now all coefficients are of order unity, indicating a reliable expansion. Moreover, all terms proportional to π^2 have cancelled. By setting $\mu = \hat{m}(\mu)$ the L terms can also be dropped. The remaining constant terms play the rôle of matching coefficients to be applied when the number of flavors in the effective theory is increased from $n_q - 1$ to n_q. This is familiar from the renormalization group evolution (RGE) of $\hat{\alpha}_s$. Since n-loop matching must be supplemented with $n+1$-loop RGE, inclusion of the $\mathcal{O}(\alpha\hat{\alpha}_s^3)$ beta function contribution is required and will be discussed later.

Eq. (3) describes the contribution of a heavy quark in the external current. The $n_q - 1$ light quarks appearing in internal loops must be treated as massless, since 3-loop diagrams involving two massive quarks with different masses have not been computed. It is indeed safe to neglect terms of $\mathcal{O}(\hat{\alpha}_s^2\hat{m}_l^2/\hat{m}_h^2)$, since in practice the heavy quark mass, $\hat{m}_h$, is always sufficiently larger than all lighter quark masses, $\hat{m}_l$, and we will follow this approximation throughout. Conversely, in $\mathcal{O}(\hat{\alpha}_s^2)$ the heavy quark also appears as a loop insertion into a one-gluon exchange diagram (the "double bubble" diagram), and in the wave function renormalization of a light quark in the external current. The limit $q^2 \to 0$ can only be performed when the heavy quark is decoupled, i.e., the $\hat{\alpha}_s$ definition for $n_q - 1$ active flavors is used. This has been done in Ref. [14],

$$\delta\hat{\Pi}^{(h)}(0) = \sum_l \frac{Q_l^2}{4\pi^2}\frac{\hat{\alpha}_s^2}{\pi^2}\left(\frac{295}{1296} - \frac{11}{72}L + \frac{L^2}{12}\right). \quad (4)$$

Eqs. (3) and (4) carry to $\mathcal{O}(\hat{\alpha}_s^2)$ the decoupling of a heavy quark [14], as was first suggested by Marciano and Rosner [15] for the case of the top quark and generalized to $\mathcal{O}(\hat{\alpha}_s)$ in Ref. [16]. The same decoupling can also be applied to the $\overline{\rm MS}$ definition of the weak mixing angle.

With $\hat{\alpha}_s(\hat{m}_c)/\pi \approx 0.13$ and the absence of non-perturbative effects, Eqs. (3) and (4) can be used reliably not only for b but also for c quarks. Complications with J/Ψ and Υ resonances are then completely avoided at the expense of the introduction of a stronger dependence on the quark masses. The numerical uncertainty due to $\hat{m}_b$ will turn out to be small, while $\hat{m}_c$ will introduce an error comparable to the one introduced through the J/Ψ resonances in the SDR approach.

III. LIGHT QUARKS

I now turn to the three light quark flavors. Applying Cauchy's theorem to the contour in Fig. 1, yields

$$\hat{\Pi}(0) = \frac{1}{\pi}\int_{4m_\pi^2}^{\mu_0^2} \frac{ds}{s - i\epsilon}\,{\rm Im}\,\hat{\Pi}(s) + \frac{1}{2\pi i}\oint_{|s|=\mu_0^2} \frac{ds}{s}\hat{\Pi}(s). \quad (5)$$

The optical theorem applied to the first term, and the substitution $s = \mu_0^2 e^{i\theta}$ to the second, brings the UDR into its final form,

$$\hat{\Pi}^{(3)}(0) = \frac{1}{12\pi^2}\int_{4m_\pi^2}^{\mu_0^2} \frac{ds}{s - i\epsilon}R(s) + \frac{1}{2\pi}\int_0^{2\pi} d\theta\,\hat{\Pi}^{(3)}(\theta). \quad (6)$$

As in the SDR approach, the first integral can be evaluated using the measured function $R(s)$ up to a scale μ_0 where PQCD is trusted. Together with the second (called $I^{(3)}$ hereafter) this results for $\mu_0 < M_{J/\Psi}$ in the 3-flavor definition $\hat{\alpha}^{(3)}(\mu_0)$. Other values of μ are obtained using RGE, and other quark and lepton flavors are included at $\mu = \hat{m}(\mu)$ using the matching description discussed before. Special care is needed if $\mu_0 > \hat{m}_c$, where conventionally 4-flavor QCD is used. The clash with 3-flavor QED will generate some extra (non-decoupling) logarithms.

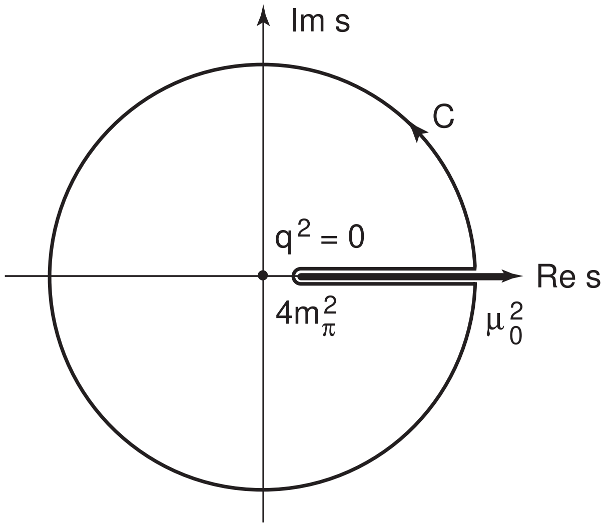

FIG. 1. Contour for an unsubtracted dispersion integration.

Indeed, following Refs. [3,4] I will use $\mu_0 = 1.8$ GeV and the result of Ref. [5], as quoted in Ref. [3],

$$\frac{\alpha M_Z^2}{3\pi} \int_{4m_\pi^2}^{\mu_0^2} ds \frac{R(s)}{s(M_Z^2 - s) - i\epsilon} = (56.9 \pm 1.1) \times 10^{-4}. \quad (7)$$

The difference between this and the first integral in Eq. (6) (times $4\pi\hat{\alpha}$) can be neglected since,

$$\frac{\alpha}{3\pi} \int_{4m_\pi^2}^{\mu_0^2} ds R(s) \left[\frac{1}{s - i\epsilon} - \frac{M_Z^2}{s(M_Z^2 - s) - i\epsilon} \right] =$$

$$2\alpha\mu_0^2 \int_0^{2\pi} d\theta \frac{\hat{\Pi}^{(3)}(\mu_0^2 e^{i\theta})}{M_Z^2 e^{-i\theta} - \mu_0^2} \approx -\frac{2\alpha\mu_0^2}{3\pi M_Z^2} \approx -6 \times 10^{-7}.$$

The second integral in Eq. (6) can again be obtained with the help of Ref. [12],

$$I^{(3)} = \frac{1}{6\pi^2} \left\{ \frac{5}{3} + \frac{\hat{\alpha}_s}{\pi} \left[\frac{55}{12} - 4\zeta(3) + 2\frac{\hat{m}_s^2(\mu_0)}{\mu_0^2} \right] + \right. \quad (8)$$

$$\left. \frac{\hat{\alpha}_s^2}{\pi^2} \left[\frac{34525}{864} - \frac{9}{4}\zeta(2) - \frac{715}{18}\zeta(3) + \frac{25}{3}\zeta(5) + F(\frac{\mu_0^2}{\hat{m}_c^2}) \right] \right\},$$

where in the $\mathcal{O}(\hat{\alpha}_s)$ term I kept the small s quark mass effect ($\sim 2 \times 10^{-6}$). $F(x)$ can be reconstructed from the absorbtive part of $\hat{\Pi}^{(3)}(s)$, i.e., $R(s)$. Below threshold it can be well approximated as an expansion in x, despite the fact that $\hat{m}_c^2 < \mu_0^2$, as can be shown by comparison with the exact result [17] (the large quark mass expansion in $\mathcal{O}(\hat{\alpha}_s^3)$ is also known [18]). The coefficients in $F(x)$ decrease even more rapidly than in $R(s)$,

$$F(x) \approx \ln x \left[\frac{2}{3}\zeta(3) - \frac{11}{12} + \frac{\ln x}{12} \right] - x \left[\frac{2}{25} - \frac{2}{135} \ln x \right]$$

$$+ x^2 \left[\frac{1513}{2116800} - \frac{\ln x}{5040} \right] - x^3 \left[\frac{1853}{80372250} - \frac{\ln x}{127575} \right].$$

In principle, $F(x)$ also applies to the tiny b quark contribution to $\hat{\Pi}^{(3)}(0)$, but without the non-decoupling logarithms in the first term.

IV. RENORMALIZATION GROUP EVOLUTION

The QED β function including QCD corrections reads,

$$\beta \equiv \mu^2 \frac{d\hat{\alpha}}{d\mu^2} = 4\pi\hat{\alpha}^2 \mu^2 \frac{d\,\hat{\Pi}(0)}{d\mu^2} \equiv -\frac{\hat{\alpha}^2}{\pi}(\beta_0 + \beta_1 \frac{\hat{\alpha}}{\pi} + \hat{\beta}_2 \frac{\hat{\alpha}^2}{\pi^2}$$

$$+ \delta_1 \frac{\hat{\alpha}_s}{\pi} + \hat{\delta}_2 \frac{\hat{\alpha}_s^2}{\pi^2} + \hat{\delta}_3 \frac{\hat{\alpha}_s^3}{\pi^3} + \hat{\delta}_4 \frac{\hat{\alpha}_s^4}{\pi^4} + \epsilon_2 \frac{\hat{\alpha}}{\pi} \frac{\hat{\alpha}_s}{\pi} + \ldots), \quad (9)$$

where coefficients with a caret are scheme dependent.

$$\beta_0 = -\sum_f \frac{Q_f^2}{3}, \quad \beta_1 = -\sum_f \frac{Q_f^4}{4}, \quad \delta_1 = -N_c C_F \sum_q \frac{Q_q^2}{4},$$

and ϵ_2 are scheme independent and can be gleaned from the 3-loop β function for simple groups [19]. $\hat{\delta}_2$ is straightforwardly computed from Eq. (3), resulting in

$$\hat{\delta}_2 = N_c C_F \sum_q Q_q^2 \left[\frac{1}{32} C_F - \frac{133}{576} C_A + \frac{11}{144} T_F n_q \right], \quad (10)$$

where for QCD we have $N_c = C_A = 3$, $C_F = 4/3$, and $T_F = 1/2$. ϵ_2 can be obtained from the first term with the substitution $Q_q^2 C_F \to Q_q^4$. The coefficients in the first and the last term of Eq. (10) are familiar from

$$\hat{\beta}_2 = \frac{1}{32} \sum_f Q_f^6 + \frac{11}{144} \left(\sum_f Q_f^4 \right) \left(\sum_f Q_f^2 \right).$$

On the other hand, the second term cannot be obtained from Refs. [19], since it cannot be disentangled from contributions with gluons in the external current. $\hat{\delta}_3$ has been obtained by Chetyrkin [20], and can also be reconstructed in the following way. Analytical continuation encodes the 4-loop order logarithms of $\hat{\Pi}(0)$ in

$$R(s) = N_c \sum_q Q_q^2 \sum_i r_i \frac{\hat{\alpha}_s^i}{\pi^i},$$

where the r_i are the non-singlet coefficients (singlet contributions which are to be treated likewise are ignored for the moment). Denoting QCD β function coefficients by $\beta_i^{(3)}$, and the constant terms appearing in Eq. (8) in two and three-loop order by $\rho_2 = C_F(55/16 - 3\zeta(3))$ and ρ_3, I find from a comparative analysis of leading logarithms in the SDR and UDR approaches,

$$\frac{\hat{\delta}_2}{\delta_1} = r_2 - \beta_0^{(3)} \rho_2, \qquad \frac{\hat{\delta}_3}{\delta_1} = r_3 - \beta_1^{(3)} \rho_2 - 2\beta_0^{(3)} \rho_3. \quad (11)$$

With the r_i from Refs. [18,21] I confirm Eq. (10), and find,

$$\hat{\delta}_3 = N_c C_F \sum_q Q_q^2 \left[\frac{23}{128} C_F^2 - \left(\frac{215}{864} - \frac{11}{72}\zeta(3) \right) C_F C_A \right.$$
$$- \left(\frac{5815}{62208} + \frac{11}{72}\zeta(3) \right) C_A^2 + \left(\frac{169}{864} - \frac{11}{36}\zeta(3) \right) C_F T_F n_q$$
$$\left. + \left(\frac{769}{15552} + \frac{11}{36}\zeta(3) \right) C_A T_F n_q + \frac{77}{3888} T_F^2 n_q^2 \right]$$
$$- \left(\sum_q Q_q \right)^2 \left(\frac{11}{144} - \frac{1}{6}\zeta(3) \right) T_F^2 d^{abc} d_{abc}, \qquad (12)$$

where for QCD $T_F^2 d^{abc} d_{abc} = 10/3$. Eqs. (10) and (12) agree with Ref. [20]. Some of the terms in Eq. (12) can also be checked with the four-loop QCD β function [22]. There are delicate cancellations for $n_q = 4$ and 5, for which $\hat{\delta}_3 = -1.21$ and 1.23, respectively (for 6 quarks $\hat{\delta}_3 = 5.79$), and the next order might be larger without this being an indication of a breakdown of perturbation theory. By assuming no cancellations in $\hat{\delta}_4$, a conservative estimate of higher order RGE contributions is $|\hat{\delta}_4/\delta_1| \leq C_A^3$. With

$$c_i = \frac{\beta_i^{(3)}}{\beta_0^{(3)}}, \quad a_0 = \frac{\hat{\alpha}_s(\mu_0)}{\pi}, \quad L = \ln \frac{\mu^2}{\mu_0^2}, \quad X = a_0 \beta_0^{(3)} L,$$

and the approximation,

$$Y = \ln(1+X) \lesssim \mathcal{O}(1), \qquad (13)$$

Eq. (9) can be solved analytically, which is welcome for numerical implementations:

$$\frac{\pi}{\hat{\alpha}(\mu)} - \frac{\pi}{\hat{\alpha}(\mu_0)} = \beta_0 L + \frac{\beta_1}{\beta_0} \ln(1 + \frac{\hat{\alpha}(\mu_0)}{\pi} \beta_0 L) + \frac{\delta_1}{\beta_0^{(3)}} Y +$$
$$\frac{1}{\beta_0^{(3)}} \frac{a_0}{1+X} [\hat{\delta}_2 X + \delta_1 c_1 (Y - X)] + \frac{1}{\beta_0^{(3)}} \left(\frac{a_0}{1+X} \right)^2 \times$$
$$[(\hat{\delta}_3 - \hat{\delta}_2 c_1)(X + \frac{X^2}{2}) + \delta_1 (c_1^2 - c_2) \frac{X^2}{2} + \hat{\delta}_2 c_1 Y - \delta_1 c_1^2 \frac{Y^2}{2}].$$

Effects from $\hat{\beta}_2 \approx 2$, and $\epsilon_2 \approx 0.05$, are well below 10^{-6}, and can be ignored. QED corrections to the QCD β function induce a contribution which is formally of the same order as ϵ_2. It turns out to be negligible, as well.

V. OTHER CONTRIBUTIONS

To complete the calculation of $\hat{\alpha}(\mu_0)$, non-hadronic contributions have to be added to Eq. (6),

$$\hat{\Pi}^{(\mathrm{non-had})}(0) = \frac{1}{4\pi^2} \left\{ \left(\frac{1}{3} + \frac{\hat{\alpha}}{4\pi} \right) \left(\ln \frac{\mu_0^2}{m_e^2} + \ln \frac{\mu_0^2}{m_\mu^2} \right) \right.$$
$$\left. + \frac{\hat{\alpha}^2}{24\pi^2} \left(\ln^2 \frac{\mu_0^2}{m_e^2} + 3 \ln^2 \frac{\mu_0^2}{m_\mu^2} \right) + \frac{15}{8} - \frac{1}{6} \right\}. \qquad (14)$$

The logarithms are the RGE effects of electrons and muons up to $\mathcal{O}(\hat{\alpha}^3)$. For consistency, only the leading logarithms should be included in 3-loop order. Leptonic $\mathcal{O}(\hat{\alpha}^3)$ results are also available in the literature [23]. The third term is the corresponding matching effect analogous to the 13/12 term in Eq. (3). At this point I should stress that $\overline{\mathrm{MS}}$ masses are used only as far as QCD is concerned; when quark effects (or leptons) get QED corrected, the mass is treated as on-shell. The last term is the bosonic contribution [16,24] (the $W^\pm$ contribution to β_0 is $+7/4$). $\mathcal{O}(\hat{\alpha}^2)$ correction are included for fermions, but not for bosons, because 2-loop electroweak calculations are generally unavailable.

VI. NON-PERTURBATIVE EFFECTS

Thus far the discussion has been entirely within perturbation theory. As stated in the introduction, non-perturbative contributions are expected to be small. In this section I will discuss the uncertainties associated with possible non-perturbative effects.

The operator product expansion (OPE) [25,26] supplements perturbation theory with terms suppressed by powers of s. Dimension 2 terms can only arise from an expansion in the light quark masses. Therefore, $D = 2$ operators can be treated perturbatively and the strange quark mass effect is already included in Eq. (8). Dynamical operators appear only at $D = 4$ and higher. For example, the strange quark and gluon condensates [26] are the dynamical operators of $D = 4$ and give rise to the contributions,

$$\Delta I^{(3)} = \frac{1}{6\pi^2} \frac{\hat{\alpha}_s^2}{\pi^2} \left[\frac{7\pi^2}{6} \frac{\langle m_s \bar{s} s \rangle}{\mu_0^4} - \frac{11\pi^2}{48} \frac{\langle \frac{\alpha_s}{\pi} GG \rangle}{\mu_0^4} \right], \quad (15)$$

where the condensates are of order $-m_K^2 f_\pi^2$ and Λ_{QCD}^4, respectively. Note, that these terms are suppressed by two powers of $\hat{\alpha}_s$ and therefore very small. They change $\hat{\alpha}(m_\tau)$ by about -2×10^{-7}, an effect completely negligible. Effects from up and down quark condensates are suppressed by a further factor of m_π^2/m_K^2, and quartic mass terms are tiny, as well.

As for the c and b quark contributions, Eq. (3) orginates from a heavy quark expansion and there is no quark vacuum expectation value. There is, however, a small contribution from the gluon condensate [26,27],

$$\Delta\hat{\Pi}^{(h)}(0) = \frac{Q_h^2}{4\pi^2}\left[-\frac{\pi^2}{30}\left(1+\frac{605}{162}\frac{\hat{\alpha}_s}{\pi}\right)\frac{\langle\frac{\alpha_s}{\pi}GG\rangle}{\hat{m}^4}\right], \quad (16)$$

which is negligible for b quarks, and is between -3 and -7×10^{-6} for c quarks, depending on the employed value for the condensate. This is still below other non-perturbative uncertainties discussed in the following. In conclusion, non-perturbative effects which can be described by local operators within the OPE are well under control. I will argue below, that this fact can also be used to limit possible other non-perturbative contributions.

While the OPE takes phenomenologically into account a class of non-perturbative effects, its coefficient functions are still computed by perturbative means. Therefore, it cannot fully assess truly non-perturbative effects proportional to $\exp(-\text{const}/\alpha_s)$. To discuss the validity of the OPE requires an understanding of such effects. The leading correction to the perturbative treatment at short distances is believed to be associated with the one-instanton solution [26,28]. In pure[1] QCD the density for instantons of small size, ρ, is proportional to [28,29]

$$\frac{\mathrm{d}\rho}{\rho^{2n+1}}\left(\frac{2\pi}{\alpha_s}\right)^6 e^{-\frac{2\pi}{\alpha_s}}, \quad (17)$$

where the integer $n\geq2$ can be fixed on dimensional grounds. Clearly, this density does not apply to large size instantons with $\rho\gtrsim\Lambda_{\rm QCD}^{-1}$, which contribute unsuppressed. For example, one expects a large size instanton contribution of order $\Lambda_{\rm QCD}^4$ to the gluon condensate ($n=2$). We lack a full understanding of instanton effects, but large size instanton contributions are described with the phenomenological parameters of the OPE.

When the expression (17) is integrated over ρ, one would encounter ultraviolet singularities for large enough n. This can be seen by changing the integration variable first to $\mu=\rho^{-1}$, and then to

$$\alpha_s(\mu) = \frac{\pi}{\beta_0^{(3)}\ln(\mu^2/\Lambda_{QCD}^2)}. \quad (18)$$

Inserting the lowest order β-function coefficient for pure QCD would result in ultraviolet divergences for $n\geq6$ [26] (see also Eq. (20) below). The interpretation of these divergences is that the integral is actually cut off at $\mu\sim\mu_0$, where μ_0 is the energy scale of the problem at hand. This limits the applicability of the OPE in two ways: (1) It introduces scale dependences in the matrix elements which are in conflict with the separation of short and large distance dynamics within the OPE. (2) Starting from some larger value of n there will be no suppression of higher order power terms.

In order to be able to trust results derived within the OPE, one should therefore try to limit possible small instanton contributions. The small size instanton density (17) can be integrated for small n,

$$\frac{A_n}{720}\int_0^\infty\frac{\mathrm{d}\alpha_s}{\alpha_s}\rho^{-2n}\left(\frac{2\pi}{\alpha_s}\right)^7 e^{-\frac{2\pi}{\alpha_s}}, \quad (19)$$

where the A_n are parameters of $\mathcal{O}(1)$ ($A_0=1$ by normalization). The α_s distribution is centered around $\alpha_s=\frac{\pi}{3}(1\pm\frac{1}{\sqrt{5}})$. For $\alpha_s(M_Z)=0.120$ this would correspond to instanton sizes $\rho\sim1.5$ GeV^{-1}. However, the extra suppression factor $\rho^{-2n}\sim\mu^{2n}$ effectively shifts the distribution center to smaller values:

$$\alpha_s = \frac{\pi}{3}\left(1-\frac{n}{2\beta_0^{(3)}}\right)\left(1\pm\frac{1}{\sqrt{5}}\right). \quad (20)$$

For large enough n the small instanton contribution will be dominated by the energy scale μ_0. One can thus read off the suppression factor for OPE breaking effects,

$$\frac{A}{720\alpha_s}\left(\frac{2\pi}{\alpha_s}\right)^7 e^{-\frac{2\pi}{\alpha_s}}\sim0.03A, \quad (21)$$

where A is a collective parameter again of $\mathcal{O}(1)$, and $\alpha_s=\alpha_s(\mu_0)$.

While one cannot estimate the parameters A_n, one can try to put an order of magnitude bound on A_2 using the phenomenological value of the two gluon condensate [3],

$$\langle\frac{\alpha_s}{\pi}GG\rangle\approx0.04\ \text{GeV}^4. \quad (22)$$

I will assume that it is dominated by small rather than large instantons. This assumption will allow an order of magnitude bound on small instanton effects if one ignores the possibility of large cancellations. For $n=2$ the integral (19) is contributed on average by instantons of scale $\mu_I\sim0.9$ GeV. Using that one can conclude, $A_2\lesssim0.07$.

Even assuming that small instantons are (unlike the OPE power terms appearing in $I^{(3)}$) not suppressed by further powers of $\hat{\alpha}_s/\pi$, one would find from Eq. (21) with $A=1$ a suppression factor of 3×10^{-2}. From that I infer that non-perturbative contributions to α^{-1} should be $\lesssim0.006$.

By ascribing a discrepancy in semileptonic D decay data to OPE breaking instanton effects, it has been argued [30] that instanton contributions could be as large as about 10% in $R(m_\tau)$. Contributions of this size are not excluded by the data, and would correspond to about 100% of the PQCD corrections. Therefore, I will take 50% of the PQCD correction to $I^{(3)}$ as a (conservative) uncertainty introduced by possible OPE breaking effects

[1]The inclusion of (almost) massless quarks rather extends the validity of the OPE [26].

(which are expected to be insignificant away from the real axis). This yields an uncertainty of ± 0.006 in α^{-1}, incidentally identical to the bound obtained before.

The SDR and UDR approaches are subject to the same size of non-perturbative effects, since we do not expect the relation between the on-shell and $\overline{\rm MS}$ definitions of $\alpha(M_Z)$ to be afflicted by low energy effects. Indeed, the authors in Ref. [31] fitted different oscillating curves to the $R(s)$ data around μ_0, and estimated the uncertainty to ± 0.002 in α^{-1}. This is of the same order of magnitude and smaller than the crude (and very conservative) estimate above.

VII. NUMERICAL ANALYSIS

In the numerical analysis I use $\hat{\alpha}_s(M_Z) = 0.120$ as a reference value. As mentioned earlier, no parametric error is included for $\hat{\alpha}_s$, which is regarded as a fit parameter.

There is a variety of c [32,33] and b [33,34] running quark mass determinations. The uncertainties quoted by the various authors are of similar size, but being almost entirely theoretical, rather ad hoc. Therefore it does not seem justifiable to use a weighted average, which would yield[2] $\hat{m}_c(\hat{m}_c) = 1.30 \pm 0.02$ GeV, i.e. a very small error. Instead, I determine the averages and uncertainties from the spread of the results. This is a selfconsistent treatment, as it only needs the usual assumption of normal error distribution[3]. The problem is then reduced to finding (posterior) information on a Gaussian distribution with (prior) unknown mean and variance, when given n data points (random drawings) y_i. It can be shown [35] that the marginal posterior distribution of the mean follows a Student-t distribution, which is centered at the sample mean,

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i, \tag{23}$$

and has the standard deviation,

$$\sqrt{\frac{1}{n(n-3)}\sum_{i=1}^{n}(y_i - \bar{y})^2}. \tag{24}$$

Using this method I find,

$$\hat{m}_c(\hat{m}_c) = 1.31 \pm 0.07 \text{ GeV}, \tag{25}$$
$$\hat{m}_b(\hat{m}_b) = 4.24 \pm 0.11 \text{ GeV}, \tag{26}$$

which introduce uncertainties of ± 0.019, and ± 0.002 in $\hat{\alpha}^{-1}(M_Z)$, respectively. These are added linearly since they are of similar origin. Notice, that the weighted and unweighted averages for $\hat{m}_c$ are (fortuitously) in very good agreement with each other.

The $\mathcal{O}(\hat{\alpha}_s^2)$ term in Eq. (8) is clearly dominated by the coefficient $-\beta_0^{(3)}\zeta(2)$. I will therefore use the analogous coefficient in $\mathcal{O}(\hat{\alpha}_s^3)$, $-(\beta_1^{(3)} + 2\beta_0^{(3)} r_2)\zeta(2) \approx -19$, as an estimate for the PQCD error in $I^{(3)}$, corresponding to ± 0.005 in $\hat{\alpha}^{-1}$. I note that this large coefficient is not problematic for PQCD, as terms of this type can be resummed to all orders. The total theoretical uncertainty is ± 0.009. Eq. (7) adds an experimental error of ± 0.015. A variation of $\hat{\alpha}_s$ within 0.120 ± 0.005 corresponds to $\hat{\alpha}^{-1}(M_Z) = 127.934^{-0.024}_{+0.020}$, but this will not be included in the final error.

The final result is

$$\begin{aligned} \hat{\alpha}^{-1}(m_\tau) &= 133.513 \pm 0.015 \pm 0.009 \pm 0.019, \\ \hat{\alpha}^{-1}(M_Z) &= 127.934 \pm 0.015 \pm 0.009 \pm 0.021, \end{aligned} \tag{27}$$

where the errors are experimental, theoretical, and parametric, respectively. $\hat{\alpha}^{-1}(m_\tau)$ is to be compared with an earlier estimate ~ 133.29 [36] based on an $\mathcal{O}(\alpha)$ calculation and $m_t = 45$ GeV. Using the $\mathcal{O}(\alpha\hat{\alpha}_s)$ conversion of Ref. [16] (with an $\mathcal{O}(\alpha\hat{\alpha}_s^2)$ improvement added), $\hat{\alpha}(M_Z)$ corresponds to

$$\Delta\bar{\alpha}^{(5)}_{\rm had}(M_Z) = 0.02779 \pm 0.00020. \tag{28}$$

Changing $\hat{\alpha}_s$ to 0.118 yields 0.02773 in perfect agreement with $\Delta\bar{\alpha}^{(5)}_{\rm had}(M_Z) = 0.02774 \pm 0.00017$ from Ref. [4]. Results for other values of $\mu \gtrsim \hat{m}_c$ can easily be obtained. A fit to all data using this approach yields for the Higgs mass,

$$M_H = 96^{+76}_{-46} \text{ GeV}, \tag{29}$$

compared to

$$M_H = 69^{+85}_{-43} \text{ GeV}, \tag{30}$$

from a fit to the same data set [9], but using $\bar{\alpha}(M_Z)$ from Ref. [5].

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[2]The various results are first converted to the scale invariant mass $\hat{m}(\hat{m})$, and averaged at the end.

[3]It is also assumed that the determinations are approximately uncorrelated, as the various determinations are very different. They range from quark potential methods and QCD sum rules to D decays and lattice spectroscopy.

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