

Precise determination of the top-quark on-shell mass M_t via its scale-invariant perturbative relation to the top-quark $\overline{\text{MS}}$ mass $\overline{m}_t(\overline{m}_t)^*$

Xu-Dong Huang (黄旭东)^{1†} Xing-Gang Wu (吴兴刚)^{2‡} Xu-Chang Zheng (郑绪昌)^{2§} Jiang Yan (闫江)^{2‡}
Zhi-Fei Wu (吴知非)^{2‡} Hong-Hao Ma (马鸿浩)^{3¶}

¹Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

²Department of Physics, Chongqing Key Laboratory for Strongly Coupled Physics, Chongqing University, Chongqing 401331, China

³Department of Physics, Guangxi Normal University, Guilin 541004, China

Abstract: The principle of maximum conformality (PMC) provides a systematic approach to solve the conventional renormalization scheme and scale ambiguities. Scale-fixed predictions of physical observables using the PMC are independent of the choice of renormalization scheme – a key requirement for renormalization group invariance. In this paper, we derive new degeneracy relations based on the renormalization group equations that involve both the usual β -function and the quark mass anomalous dimension γ_m -function. These new degeneracy relations enable improved PMC scale-setting procedures for correct magnitudes of the strong coupling constant and $\overline{\text{MS}}$ -running quark mass to be determined simultaneously. By using these improved PMC scale-setting procedures, the renormalization scale dependence of the $\overline{\text{MS}}$ -on-shell quark mass relation can be eliminated systematically. Consequently, the top-quark on-shell (or $\overline{\text{MS}}$) mass can be determined without conventional renormalization scale ambiguity. Taking the top-quark $\overline{\text{MS}}$ mass $\overline{m}_t(\overline{m}_t) = 162.5_{-1.5}^{+2.1}$ GeV as the input, we obtain $M_t \approx 172.41_{-1.57}^{+2.21}$ GeV. Here, the uncertainties arise from errors combined with those from $\Delta\alpha_s(M_Z)$ and the approximate uncertainty resulting from the uncalculated five-loop terms predicted through the Padé approximation approach.

Keywords: perturbative QCD, top quark mass, renormalization

DOI: 10.1088/1674-1137/ad2dbf

I. INTRODUCTION

The top quark is the heaviest elementary particle in the Standard Model (SM), and its mass is one of the most important input parameters of the SM. The largest mass among quarks, or equivalently the strongest Yukawa coupling, implies that the top quark plays a crucial role in governing the stability of the electroweak vacuum. Determining the top-quark mass accurately is helpful for testing the precision of the SM, assessing whether the vacuum is in stable or meta-stable state, and searching for new physics beyond the SM. Direct measurements of the top-quark mass exhibit high precision in proton-proton (pp) collisions at the LHC [1–8]; these measurements

rely on the reconstruction of the top quark decay products and multipurpose Monte Carlo (MC) event generators. Other measurements were also reported in Refs. [9–17]. In the theoretical side, many studies aimed to relate the top-quark mass to its on-shell (OS) scheme mass, c.f. Refs. [18–25]. A 0.5 ~ 1 GeV difference between the top-quark MC mass (M_t^{MC}) and top-quark OS mass (M_t^{OS}) has been reported [26–32].

The top-quark OS mass has been investigated in detail in Refs. [33–52]. This mass can be related to the modified minimal subtraction ($\overline{\text{MS}}$) scheme running mass by using the perturbative relations between the top-quark bare mass ($m_{t,0}$) and renormalized mass in the OS- or $\overline{\text{MS}}$ -scheme, e.g., $m_{t,0} = Z_m^{\text{OS}} M_t^{\text{OS}}$ and $m_{t,0} = Z_m^{\overline{\text{MS}}} \overline{m}_t(\mu_r)$. In

Received 18 January 2024; Accepted 26 February 2024; Published online 27 February 2024

* Supported in part by the National Natural Science Foundation of China (12247129, 12175025, 12347101) and the Graduate Research and Innovation Foundation of Chongqing, China (ydstd1912)

[†] E-mail: huangxd@ihep.ac.cn

[‡] E-mail: wuxg@cqu.edu.cn

[§] E-mail: zhengxc@cqu.edu.cn

[‡] E-mail: yjiang@cqu.edu.cn

[‡] E-mail: zfwu@cqu.edu.cn

[¶] E-mail: mahonghao@pku.edu.cn



Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Article funded by SCOAP³ and published under licence by Chinese Physical Society and the Institute of High Energy Physics of the Chinese Academy of Sciences and the Institute of Modern Physics of the Chinese Academy of Sciences and IOP Publishing Ltd

these expressions, Z_m^{OS} and $Z_m^{\overline{\text{MS}}}$ are quark mass renormalization constants in the OS- and $\overline{\text{MS}}$ -schemes, respectively. In perturbative Quantum Chromodynamics (pQCD) theory, the relation between the OS mass and $\overline{\text{MS}}$ mass has been calculated up to four-loop level [53–65]. This allows for determining the OS mass with the help of experimental results for the $\overline{\text{MS}}$ mass. In the determination process, the key issue is to set the exact values of the strong coupling constant (α_s) and $\overline{\text{MS}}$ mass (e.g., \overline{m}_q , $q = c, b, t$ denote the charm, bottom, and top quarks, respectively). The scale running behavior of α_s and \overline{m}_q is governed by general renormalization group equations (RGEs) involving both the β function and quark mass anomalous dimension γ_m :

$$\frac{d\alpha_s(\mu_r)}{d\ln\mu_r^2} = \beta(\alpha_s) = -\sum_{i=0}^{\infty} \beta_i \alpha_s^{i+2}(\mu_r), \quad (1)$$

$$\frac{d\overline{m}_q(\mu_r)}{d\ln\mu_r^2} = \overline{m}_q(\mu_r) \gamma_m(\alpha_s) = -\overline{m}_q(\mu_r) \sum_{i=0}^{\infty} \gamma_i \alpha_s^{i+1}(\mu_r), \quad (2)$$

where $a_s(\mu_r) = \alpha_s(\mu_r)/(4\pi)$. The $\{\beta_i\}$ - and $\{\gamma_i\}$ -functions have been calculated up to five-loop level in the $\overline{\text{MS}}$ -scheme [66–74], e.g., $\beta_0 = 11 - 2n_f/3$ and $\gamma_0 = 4$, where n_f is the number of active flavors. Using reference points such as $\alpha_s(M_Z) = 0.1179 \pm 0.0009$ and $\overline{m}_t(\overline{m}_t) = 162.5_{-1.5}^{+2.1}$ GeV, reported by the Particle Data Group [75], their values can be obtained at any scale.

Because of renormalization group invariance (RGI), the physical observable is independent of any choices of renormalization scheme and scale. However, for a fixed-order pQCD prediction, the mismatching of α_s and the pQCD coefficients at each order leads to the well-known renormalization scheme-and-scale ambiguities. To eliminate such artificially introduced renormalization scheme-and-scale ambiguities, the principle of maximum conformality (PMC) was proposed [76–79]. This principle sets the underlying procedure for the well-known Brodsky-Lepage-Mackenzie (BLM) method [80] as well as a rule for generalizing the BLM procedure up to all orders. A short review of the development of the PMC from the BLM method can be found in Ref. [81]. All the features previously observed in the studies on the BLM method are also adaptable to the PMC with or without proper transformations, e.g., only the RG-involved n_f -terms in the pQCD series should be treated as non-conformal

terms and be adopted for setting the correct magnitude of α_s . The PMC thus provides a rigorous scale-setting approach for obtaining unambiguous fixed-order pQCD predictions consistent with the principles of the renormalization group¹⁾. Moreover, its predictions satisfy all the requirements for renormalization group invariance [87, 88]. A complete discussion about the PMC can be found in review articles [89–91].

To date, the PMC method has been successfully applied to many high-energy processes, c.f. Refs. [92–98], aiming to determine the correct magnitude of the strong running coupling α_s of the pQCD series by using the procedures suggested in Refs. [99, 100]. However, there are also many other advances related to both the running coupling α_s and quark $\overline{\text{MS}}$ running mass \overline{m}_q . If the pQCD series contains both the n_f -terms related to the renormalization of α_s and the n_f -terms related to the renormalization of \overline{m}_q , some extra treatments must be applied before using the formulas listed in Refs. [99, 100]; those formulas are based on the assumption that both the conformal and non-conformal terms have been correctly distributed²⁾. To achieve a correct PMC prediction, the degeneracy relations among different orders, which jointly constitute a general property of the QCD theory [103], should be applied correctly. In this paper, we derive new degeneracy relations with the help of the RGEs involving both the β -function and quark mass anomalous dimension γ_m -function, which lead to improved PMC scale-setting procedures. Such procedures are then applied for determining the top-quark OS mass by simultaneously determining the correct magnitudes of α_s and quark $\overline{\text{MS}}$ running mass \overline{m}_q of the perturbative series with the help of RGEs for either the running coupling α_s or running mass.

The rest of this paper is organized as follows. In Sec. II, we describe the special degeneracy relations of the non-conformal terms in the perturbative coefficients by using the \mathcal{R}_δ -scheme. Then, we elaborate on the improved procedures of the PMC scale-setting approach under the running mass scheme. We apply these procedures in Sec. III to determine the top-quark OS mass M_t via its perturbative relation to the $\overline{\text{MS}}$ mass. Section IV presents a summary.

II. CALCULATION TECHNOLOGY

A. Observables in \mathcal{R}_δ -scheme

The \mathcal{R}_δ -scheme represents the MS-type renormaliza-

1) A practical way of achieving scheme-and-scale invariant prediction directly from the initial series, which is called as principal of minimum sensitivity (PMS) [82, 83] has been suggested in the literature. It assumes that all uncalculated higher-order terms give zero contribution and determines the optimal scheme and scale by requiring the slope of the pQCD series over scheme and scale choices vanish. Since the PMS breaks the standard renormalization group invariance [84], it thus cannot be treated as a strict solution of conventional scheme-and-scale ambiguities, which however could be treated as an effective treatment [85, 86].

2) We have observed that a study on the relation between the OS mass and the $\overline{\text{MS}}$ running mass by using the PMC has been issued in Ref. [101]. It should be pointed out that the authors there do not distinguish the functions of various n_f -terms in the perturbative series, which is however important to achieve a precise prediction [102]. Thus their treatments can only be treated as an effective but not a strict application of the PMC.

tion scheme with a subtraction term $\ln(4\pi) - \gamma_E - \delta$, where δ is an arbitrary finite number [99] satisfying that $\mathcal{R}_{\delta=0} = \overline{\text{MS}}$. As an extension of Ref. [99], we consider the pQCD prediction $\rho(Q^2)$ including the $\overline{\text{MS}}$ running mass. In the reference scheme \mathcal{R}_0 , this prediction can be expressed as follows:

$$\rho_0(Q^2) = r_0 \overline{m}_q^n(\mu_r) \left[1 + \sum_{k=1}^{\infty} r_k (\mu_r^2/Q^2) a_s^k(\mu_r) \right], \quad (3)$$

where ρ_0 denotes the pQCD prediction ρ in the \mathcal{R}_0 scheme, Q represents a physical scale of the measured observable¹⁾, \overline{m}_q is the quark $\overline{\text{MS}}$ running mass, n is the power of \overline{m}_q associated with the tree-level term, and r_0 is a global factor. For simplicity, we assume that r_0 does not have a_s . The pQCD series is independent of the choice of renormalization scale μ_r , provided that it has been calculated up to all orders. However, it is not feasible to achieve this goal owing to the difficulty of high-order calculations. Generally, the pQCD series becomes a renormalization scale that depends on the scheme at any finite order; this dependence can be exposed by using the \mathcal{R}_δ -scheme. One can derive the general expression for ρ in \mathcal{R}_δ -scheme by using the scale displacements in any \mathcal{R}_δ -scheme:

$$a_s(\mu_r) = a_s(\mu_\delta) + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{d^n a_s(\mu_r)}{(d \ln \mu_r^2)^n} \right|_{\mu_r=\mu_\delta} (-\delta)^n, \quad (4)$$

$$\overline{m}_q(\mu_r) = \overline{m}_q(\mu_\delta) + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{d^n \overline{m}_q(\mu_r)}{(d \ln \mu_r^2)^n} \right|_{\mu_r=\mu_\delta} (-\delta)^n, \quad (5)$$

where $\delta = -\ln(\mu_r^2/\mu_\delta^2)$. It is useful to derive the general displacement relations as expansions up to fixed order, as shown in Appendix A.

Inserting these scale displacements into Eq. (3), one can obtain the expression of ρ_δ for an arbitrary δ in any \mathcal{R}_δ -scheme:

$$\begin{aligned} \rho_\delta(Q^2) &= r_0 \overline{m}_q^n(\mu_\delta) \{ 1 + (r_1 + n\gamma_0 \delta) a_s(\mu_\delta) \\ &\quad + [r_2 + \beta_0 r_1 \delta + n(\gamma_1 + \gamma_0 r_1) \delta + \frac{n}{2} \beta_0 \gamma_0 \delta^2 \\ &\quad + \frac{n^2}{2} \gamma_0^2 \delta^2] a_s^2(\mu_\delta) + \mathcal{O}[a_s^3(\mu_\delta)] \}, \end{aligned} \quad (6)$$

where ρ_δ denotes the pQCD prediction ρ in the \mathcal{R}_δ scheme and $\mu_\delta^2 = \mu_r^2 e^\delta$. A useful expression of ρ_δ up to a_s^4 -order is provided in Appendix B. It is easy to return to ρ_0 by setting $\delta = 0$. A further description of the \mathcal{R}_δ -scheme

can be found in Sec. II of Ref. [99].

The renormalization group invariance requires that the perturbative series up to all orders for a physical observable be independent of the theoretical convention:

$$\begin{aligned} \frac{d\rho_\delta}{d\delta} &= \frac{\partial \rho_\delta}{\partial \delta} + \beta(a_s) \frac{\partial \rho_\delta}{\partial a_s} + \overline{m}_q \gamma_m(a_s) \frac{\partial \rho_\delta}{\partial \overline{m}_q} \\ &= 0. \end{aligned} \quad (7)$$

Thus, we can obtain

$$\frac{\partial \rho_\delta}{\partial \delta} = -\beta(a_s) \frac{\partial \rho_\delta}{\partial a_s} - \overline{m}_q \gamma_m(a_s) \frac{\partial \rho_\delta}{\partial \overline{m}_q}. \quad (8)$$

Therefore, by absorbing all $\{\beta_i\}$ and $\{\gamma_i\}$ dependences into the running coupling constant and quark running mass in Eq. (6), one can obtain a scheme-invariant prediction given that the δ -dependence is vanished. Therefore, the coefficients of the resultant series will be equal to those of the conformal (or scale-invariant) theory, that is, $\partial \rho_\delta / \partial \delta = 0$.

The expression in Eq. (6) also exposes the pattern of $\{\beta_i\}$ -terms and $\{\gamma_i\}$ -terms in the coefficients at each order. Given that there is nothing special about any particular value of δ , it is possible to infer some degenerate relations between certain coefficients of the $\{\beta_i, \gamma_i\}$ -terms from the expression ρ_δ . That is, the coefficients of $\beta_0 a_s^2$ and $n\gamma_0 a_s^2$ can be set equal, given that their coefficients are both $r_1 \delta$. Therefore, for any scheme, the expression for ρ can be transformed into a similar form to that of ρ_δ :

$$\begin{aligned} \rho(Q^2) &= r_0 \overline{m}_q^n(\mu_r) \left\{ 1 + \left(\hat{r}_{1,0} + n\gamma_0 \ln \frac{\mu_r^2}{Q^2} \right) a_s(\mu_r) \right. \\ &\quad + \left[\hat{r}_{2,0} + \beta_0 \hat{r}_{2,1} + n\gamma_0 \hat{r}_{2,1} \right. \\ &\quad + (\beta_0 \hat{r}_{1,0} + n\gamma_1 + n\gamma_0 \hat{r}_{1,0}) \ln \frac{\mu_r^2}{Q^2} \\ &\quad + \left. \frac{1}{2} (n\beta_0 \gamma_0 + n^2 \gamma_0^2) \ln^2 \frac{\mu_r^2}{Q^2} \right] a_s^2(\mu_r) \\ &\quad \left. + \mathcal{O}[a_s^3(\mu_r)] \right\}, \end{aligned} \quad (9)$$

where $\hat{r}_{i,j}$ are coefficients that do not depend on μ_r , $\hat{r}_{i,0}$ are conformal coefficients, and the $\{\beta_i, \gamma_i\}$ -terms are non-conformal terms. A useful expression up to a_s^4 -order is provided in Appendix C. It is easy to find the relationships between the coefficients $r_k(\mu_r^2/Q^2)$ and $\hat{r}_{i,j}$:

1) The Q represents the typical physical scale of the measured observable, which always appears in the pQCD calculation associated with μ_r . For example, in the calculation of the n -loop pQCD correction to the cross section of $e^+(k_1) + e^-(k_2) \rightarrow \gamma^* \rightarrow q(k_3) + \bar{q}(k_4)$, the calculated results include terms like $\ln(\mu_r^2/s)$ where $s = (k_1 + k_2)^2 = (k_3 + k_4)^2$ represents the squared center-of-mass energy. Thus, the scale Q appears in the expression automatically as $Q = \sqrt{s}$.

$$r_1(\mu_r^2/Q^2) = \hat{r}_{1,0} + n\gamma_0 \ln \frac{\mu_r^2}{Q^2}, \quad (10)$$

$$\begin{aligned} r_2(\mu_r^2/Q^2) &= \hat{r}_{2,0} + \beta_0 \hat{r}_{2,1} + n\gamma_0 \hat{r}_{2,1} \\ &\quad + (\beta_0 \hat{r}_{1,0} + n\gamma_1 + n\gamma_0 \hat{r}_{1,0}) \ln \frac{\mu_r^2}{Q^2} \\ &\quad + \frac{1}{2} (n\beta_0 \gamma_0 + n^2 \gamma_0^2) \ln^2 \frac{\mu_r^2}{Q^2}, \end{aligned} \quad (11)$$

The relationships between the coefficients $r_k(\mu_r^2/Q^2)$ ($k = 3, 4$) and $\hat{r}_{i,j}$ are provided in Appendix D. These relationships lead to systematic procedures to determine the coefficients $\hat{r}_{i,j}$. In some cases, the coefficients $r_k(\mu_r^2/Q^2)$ in Eq. (3) are computed numerically, and the $\{\beta_i, \gamma_i\}$ dependence is not known explicitly. However, it is straightforward to obtain the dependence on the number of quark flavors n_f , because n_f enters analytically in any loop diagram computation. To apply the PMC scale-setting approach, one should put the pQCD expression into the form of Eq. (9). Owing to the special degeneracy relations in the coefficients of $\{\beta_i, \gamma_i\}$ -terms, the n_f series can be matched to the $\hat{r}_{i,j}$ coefficients in a unique manner. The k_{th} -order coefficient in pQCD has an expansion in n_f that reads

$$r_k(\mu_r^2/Q^2) = c_{k,0} + c_{k,1}n_f + \dots + c_{k,k-1}n_f^{k-1}, \quad (12)$$

where the coefficients $c_{k,l}$ are obtained from the pQCD calculation and are a function of μ_r and Q . Then, the coefficients $\hat{r}_{i,j}$ in Eq. (9) can be determined by using their relationship with $r_k(\mu_r^2/Q^2)$ and the known coefficients $c_{k,l}$. The steps are detailed in Appendix E. In the next section, we will show improved PMC formulas under the running mass scheme.

B. PMC single-scale approach under the running mass scheme

Adopting the PMC single-scale approach [100], the overall effective running coupling $a_s(Q_*)$ and effective running mass $\bar{m}_q(Q_*)$ can be determined by absorbing all the non-conformal terms. Eq. (9) transforms into the following conformal series:

$$\begin{aligned} \rho(Q^2) &= r_0 \bar{m}_q^n(Q_*) \{1 + \hat{r}_{1,0} a_s(Q_*) + \hat{r}_{2,0} a_s^2(Q_*) \\ &\quad + \hat{r}_{3,0} a_s^3(Q_*) + \hat{r}_{4,0} a_s^4(Q_*) + \mathcal{O}[a_s^5(Q_*)]\}, \end{aligned} \quad (13)$$

where Q_* is the PMC scale. More explicitly, by using the scale displacement relations to shift the scale μ_r to Q_* in Eq. (9), the PMC scale Q_* can be determined by requiring that all non-conformal terms (NonConf.) vanish:

$$\begin{aligned} \rho(Q^2)_{\text{NonConf.}} &= r_0 \bar{m}_q^n(Q_*) \{r_{1,\text{NonConf.}}(Q_*) a_s(Q_*) \\ &\quad + r_{2,\text{NonConf.}}(Q_*) a_s^2(Q_*) \\ &\quad + r_{3,\text{NonConf.}}(Q_*) a_s^3(Q_*) \\ &\quad + r_{4,\text{NonConf.}}(Q_*) a_s^4(Q_*) + \mathcal{O}[a_s^5(Q_*)]\} \\ &= 0, \end{aligned} \quad (14)$$

where

$$r_{1,\text{NonConf.}}(Q_*) = n\gamma_0 \ln \frac{Q_*^2}{Q^2}, \quad (15)$$

$$\begin{aligned} r_{2,\text{NonConf.}}(Q_*) &= \beta_0 \hat{r}_{2,1} + n\gamma_0 \hat{r}_{2,1} \\ &\quad + (\beta_0 \hat{r}_{1,0} + n\gamma_1 + n\gamma_0 \hat{r}_{1,0}) \ln \frac{Q_*^2}{Q^2} \\ &\quad + \frac{1}{2} (n\beta_0 \gamma_0 + n^2 \gamma_0^2) \ln^2 \frac{Q_*^2}{Q^2}, \end{aligned} \quad (16)$$

where the higher-order coefficients $r_{i,\text{NonConf.}}$ ($i = 3, 4$) are provided in Appendix F.

Owing to its perturbative nature, the solution of $\ln(Q_*^2/Q^2)$ can be expanded as a power series over $a_s(Q_*)$:

$$\ln \frac{Q_*^2}{Q^2} = \sum_{i=0}^n S_i a_s^i(Q_*), \quad (17)$$

where S_i are perturbative coefficients that can be derived by solving Eq. (14). For $n \neq 0$, the first three coefficients S_i ($i = 0, 1, 2$) are

$$S_0 = 0, \quad (18)$$

$$S_1 = -\frac{(\beta_0 + n\gamma_0) \hat{r}_{2,1}}{n\gamma_0}, \quad (19)$$

$$\begin{aligned} S_2 &= \hat{r}_{1,0} \hat{r}_{2,1} - \hat{r}_{3,1} - \frac{n\gamma_0 \hat{r}_{3,2}}{2} - \frac{\beta_1 \hat{r}_{2,1}}{n\gamma_0} \\ &\quad + \beta_0 \left(\frac{\gamma_1 \hat{r}_{2,1}}{n\gamma_0^2} + \frac{2\hat{r}_{1,0} \hat{r}_{2,1} - 2\hat{r}_{3,1}}{n\gamma_0} - \frac{3\hat{r}_{3,2}}{2} \right) \\ &\quad + \beta_0^2 \left(\frac{\hat{r}_{1,0} \hat{r}_{2,1}}{n^2 \gamma_0^2} - \frac{\hat{r}_{3,2}}{n\gamma_0} \right), \end{aligned} \quad (20)$$

and S_3 is provided in Appendix G. Following this idea, the PMC scale Q_* can be fixed at any order; the correct magnitudes of the quark running mass \bar{m}_q and running coupling constant a_s are determined simultaneously. Matching the μ_r -independent conformal coefficients $\hat{r}_{i,0}$, the resultant PMC series will be free of conventional renormalization scale ambiguity. In the following section, we apply these formulas to determine the top-quark OS

mass M_t via its perturbative relation to the $\overline{\text{MS}}$ mass.

III. NUMERICAL RESULTS

For numerical calculations, we adopted $\alpha_s(M_Z) = 0.1179 \pm 0.0009$ and $\overline{m}_t(\overline{m}_t) = 162.5^{+2.1}_{-1.5}$ GeV [75]. The running of the strong coupling $\alpha_s(\mu_r)$ was evaluated using the RunDec program [104].

A. Properties of the top-quark on-shell mass M_t

The relation between the $\overline{\text{MS}}$ quark mass and OS quark mass can be expressed as

$$\frac{\overline{m}_t(\mu_r)}{M_t} = \frac{Z_m^{\text{OS}}}{Z_m^{\overline{\text{MS}}}} = \sum_{n \geq 0} a_s^n(\mu_r) z_m^{(n)}(\mu_r), \quad (21)$$

where $z_m^{(0)}(\mu_r) = 1$ and $z_m^{(n)}(\mu_r)$ is a function of $\ln(\mu_r^2/M_t^2)$. As an expansion of a previous study [95], we focus on the inverted relation with respect to Eq. (21),

$$\frac{M_t}{\overline{m}_t(\mu_r)} = \frac{Z_m^{\overline{\text{MS}}}}{Z_m^{\text{OS}}} = \sum_{n \geq 0} a_s^n(\mu_r) c_m^{(n)}(\mu_r), \quad (22)$$

where $c_m^{(0)}(\mu_r) = 1$ and $c_m^{(n)}(\mu_r)$ is a function of $\ln(\mu_r^2/\overline{m}_t^2(\mu_r))$. Then, we can determine the top-quark OS mass using the following relationship:

$$M_t = \overline{m}_t(\mu_r) \{1 + r_1(\mu_r) a_s(\mu_r) + r_2(\mu_r) a_s^2(\mu_r) + r_3(\mu_r) a_s^3(\mu_r) + r_4(\mu_r) a_s^4(\mu_r) + \mathcal{O}[a_s^5(\mu_r)]\}, \quad (23)$$

where the perturbative coefficients $r_i(\mu_r)$ ($i = 1, 2, 3, 4$) were reported in Refs. [61, 62] and $r_i(\mu_r)$ are functions of $\ln(\mu_r^2/\overline{m}_t^2(\mu_r))$. The μ_r dependence of the top-quark $\overline{\text{MS}}$ running mass $\overline{m}_t(\mu_r)$ is governed by the quark mass anomalous dimension γ_m , which has been calculated up to $\mathcal{O}(\alpha_s^5)$ [71, 72]. Thus, the top-quark $\overline{\text{MS}}$ running mass $\overline{m}_t(\mu_r)$ can be determined by the following equation [72]:

$$\overline{m}_t(\mu_r) = \overline{m}_t(\overline{m}_t) \frac{c_t[\alpha_s(\mu_r)/\pi]}{c_t[\alpha_s(\overline{m}_t)/\pi]}, \quad (24)$$

where $c_t[x] = x^{4/7} (1 + 1.19796x + 1.79348x^2 - 0.683433x^3 - 3.53562x^4)$.

By setting all input parameters to their central values, the top-quark OS mass M_t under the conventional scale-setting approach can be represented as depicted in Fig. 1. In particular, Fig. 1 shows that, in agreement with conventional wisdom, the renormalization scale dependence of conventional series becomes smaller when more loop terms have been included. Numerically, we have $M_t|_{\text{Conv.}}^{\mathcal{O}(\alpha_s^4)} = [172.23, 172.88]$ for $\mu_r \in [\overline{m}_t(\overline{m}_t)/2, 2\overline{m}_t(\overline{m}_t)]$; e.g., the net scale uncertainty becomes $\sim 0.4\%$ for a α_s^4 -order

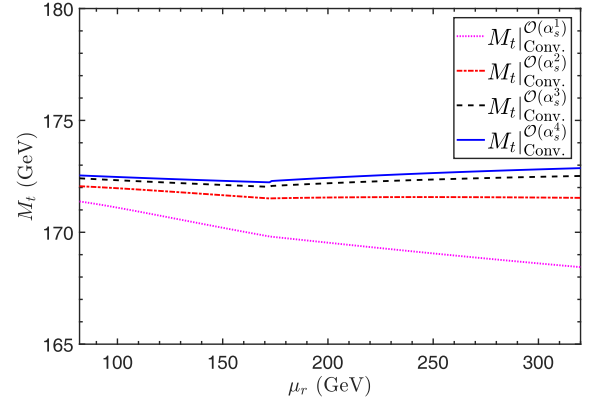


Fig. 1. (color online) Top-quark OS mass M_t versus renormalization scale (μ_r) under the conventional scale-setting approach up to different perturbative orders.

correction. This small net scale dependence for the prediction up to α_s^4 -order is due to the well convergent behavior of the perturbative series. The relative magnitudes among different orders change significantly for different choices of μ_r ; for example, the relative magnitudes of the leading-order-terms (LO): next-to-leading-order-terms (NLO): next-to-next-to-leading-order-terms (N^2LO): next-to-next-to-next-to-leading-order-terms (N^3LO): next-to-next-to-next-to-next-to-leading-order-terms (N^4LO) $\simeq 1: 4.60\%: 0.98\%: 0.30\%: 0.12\%$ for $\mu_r = \overline{m}_t(\overline{m}_t)$, which represents a proper perturbative nature. More specifically, M_t up to N^4LO -level has the following perturbative behavior:

$$\begin{aligned} M_t|_{\text{Conv.}} &= 162.5_{-0.83}^{-8.15} + 7.48_{+0.62}^{+6.36} + 1.60_{+0.14}^{+1.80} \\ &\quad + 0.49_{+0.03}^{+0.47} + 0.19_{+0.01}^{+0.14} \\ &= 172.26_{-0.03}^{+0.62} \text{ (GeV)}, \end{aligned} \quad (25)$$

whose central values are those for $\mu_r = \overline{m}_t(\overline{m}_t)$, and the scale uncertainties are estimated by varying $\mu_r \in [\overline{m}_t(\overline{m}_t)/2, 2\overline{m}_t(\overline{m}_t)]$. The higher-order prediction of M_t is not a monotonic function of μ_r , which leads to asymmetric uncertainty. By using another usual choice, i.e., $\mu_r = 172.5$ GeV, and varying this value within the range of $[1/2 \times 172.5, 2 \times 172.5]$, we obtain $M_t = 172.29_{-0.06}^{+0.64}$ GeV. The central value shifts from 172.26 GeV by $+0.03$ GeV, and its uncertainty remains asymmetric.

We present M_t under PMC scale-setting approach in Fig. 2, which shows the top-quark OS mass M_t under the PMC single-scale approach up to different perturbative orders:

$$M_t|_{\text{PMC}}^{\mathcal{O}(\alpha_s^4)} = \{170.01, 172.66, 172.27, 172.41\} \text{ (GeV)} \quad (26)$$

for $n = 1, 2, 3$, and 4, respectively. There is no renormalization scale ambiguity for the PMC prediction, and M_t

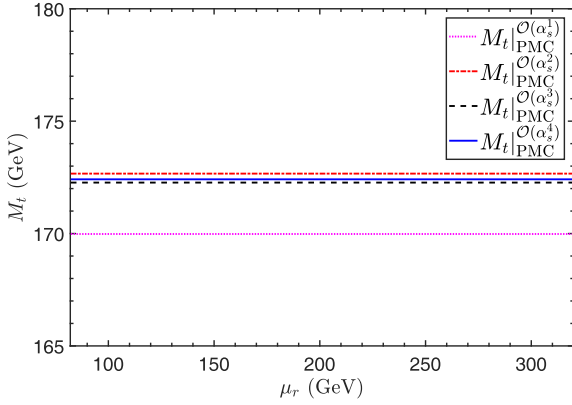


Fig. 2. (color online) Top-quark OS mass M_t versus renormalization scale (μ_r) under the PMC single-scale approach up to different perturbative orders.

quickly approaches its steady value. After applying the PMC, the perturbative nature of the M_t pQCD series is notably improved owing to the elimination of divergent renormalization terms. Moreover, the relative importance of the LO-terms: NLO-terms: N²LO-terms: N³LO-terms: N⁴LO-terms changes to 1: 4.79%: -1.15%: -0.15%: 0.07%. Up to N⁴LO-level, we have

$$\begin{aligned} M_t|_{\text{PMC}} &= \bar{m}_t(Q_*) \{1 + \hat{r}_{1,0} a_s(Q_*) + \hat{r}_{2,0} a_s^2(Q_*) \\ &\quad + \hat{r}_{3,0} a_s^3(Q_*) + \hat{r}_{4,0} a_s^4(Q_*) + O[a_s^5(Q_*)]\} \\ &= 166.49 + 7.97 - 1.92 - 0.25 + 0.12 \\ &= 172.41 \text{ (GeV)}, \end{aligned} \quad (27)$$

where the PMC scale Q_* can be established up to next-to-next-to-leading-log (N²LL) accuracy by using Eq. (17) as follows:

$$\begin{aligned} \ln \frac{Q_*^2}{\bar{m}_t^2(Q_*)} &= -68.73 a_s(Q_*) + 247.483 a_s^2(Q_*) \\ &\quad - 6447.27 a_s^3(Q_*), \end{aligned} \quad (28)$$

which leads to $Q_* = 123.3$ GeV. Owing to its perturbative nature, we take the magnitude of the last known term as the unknown N³LL term in a conservative estimation of the unknown perturbative terms. Thus, we obtain a scale shift of $\Delta Q_* = \begin{pmatrix} +0.2 \\ -0.3 \end{pmatrix}$ GeV, which leads to

$$\Delta M_t|_{\text{PMC}} = \begin{pmatrix} +0.04 \\ -0.03 \end{pmatrix} \text{ (GeV)}. \quad (29)$$

This uncertainty can be defined as *the first type of residual scale dependence due to unknown higher-order terms* [105]. Such residual scale dependence is distinct from the conventional scale ambiguities and is sup-

pressed owing to the perturbative nature of the PMC scale. For the present case, the residual scale dependence expressed by Eq. (29) is much smaller than the conventional scale uncertainty presented in Eq. (25).

B. Theoretical uncertainties

In pQCD calculations, the magnitude of unknown perturbative terms is also a major source of uncertainty. It is helpful to find a reliable prediction of the unknown higher-order terms. The Padé approximation approach (PAA) [106, 107] is a well-known method to estimate the $(n+1)$ _{th}-order coefficient for a given n _{th}-order perturbative series; this method has been tested on various known QCD results [108]. More explicitly, for the pQCD approximant $\rho(Q^2) = c_1 a_s + c_2 a_s^2 + c_3 a_s^3 + c_4 a_s^4$, the preferable $[n/n+1]$ -type PAA prediction [109] of the a_s^5 -terms of M_t under the conventional scale-setting approach is

$$\rho_{[1/2]}^{\text{N}^5\text{LO}} = \frac{2c_2 c_3 c_4 - c_3^2 - c_1 c_4^2}{c_2^2 - c_1 c_3} a_s^5, \quad (30)$$

whereas the preferable $[0/n-1]$ -type PAA prediction of the a_s^5 -terms of M_t under the PMC scale-setting approach [92] is

$$\rho_{[0/3]}^{\text{N}^5\text{LO}} = \frac{c_2^4 - 3c_1 c_2^2 c_3 + 2c_1^2 c_2 c_4 + c_1^2 c_3^2}{c_1^3} a_s^5. \quad (31)$$

This uncertainty can be defined as *the second type of residual scale dependence* due to unknown higher-order terms. Then, our prediction of the magnitude of the N⁵LO-terms of top-quark OS mass M_t is

$$\Delta M_t|_{\text{Conv.}}^{\text{N}^5\text{LO}} = \pm 0.08 \text{ (GeV)}, \quad (32)$$

$$\Delta M_t|_{\text{PMC}}^{\text{N}^5\text{LO}} = \pm 0.02 \text{ (GeV)}. \quad (33)$$

Note that the conventional result is obtained by setting $\mu_r = \bar{m}_t(\bar{m}_t)$, leading to numerical values that vary with the renormalization scale owing to the fact that the coefficients c_i are not fixed at each order. However, the PAA prediction of the PMC series exhibits no renormalization scale ambiguity, given that the PMC coefficients are scale-invariant.

The combination of the two aforementioned residual scale dependences leads to a net perturbative uncertainty due to uncalculated higher-order terms under conventional and PMC scale-setting approaches:

$$\Delta M_t|_{\text{Conv.}}^{\text{High order}} = \begin{pmatrix} +0.63 \\ -0.09 \end{pmatrix} \text{ (GeV)}, \quad (34)$$

$$\Delta M_t|_{\text{PMC}}^{\text{High order}} = \pm 0.04 \text{ (GeV)}. \quad (35)$$

This shows that the PMC scale-invariant series provides a more accurate basis than the conventional scale-dependent series for estimating the uncertainty caused by uncalculated higher-order terms.

There are uncertainties from $\Delta\alpha_s(M_Z)$ and $\Delta\bar{m}_t(\bar{m}_t)$. As an estimation, setting $\Delta\alpha_s(M_Z) = \pm 0.0009$ [75], we obtain

$$\Delta M_t|_{\text{Conv.}}^{\Delta\alpha_s(M_Z)} = \pm 0.09 \text{ (GeV)}, \quad (36)$$

$$\Delta M_t|_{\text{PMC}}^{\Delta\alpha_s(M_Z)} = \begin{pmatrix} +0.10 \\ -0.08 \end{pmatrix} \text{ (GeV)}. \quad (37)$$

To estimate the uncertainty from the top-quark $\overline{\text{MS}}$ mass, setting $\Delta\bar{m}_t(\bar{m}_t) = \begin{pmatrix} +2.1 \\ -1.5 \end{pmatrix}$ GeV, we obtain

$$\Delta M_t|_{\text{Conv.}}^{\Delta\bar{m}_t(\bar{m}_t)} = \begin{pmatrix} +2.20 \\ -1.57 \end{pmatrix} \text{ (GeV)}, \quad (38)$$

$$\Delta M_t|_{\text{PMC}}^{\Delta\bar{m}_t(\bar{m}_t)} = \begin{pmatrix} +2.21 \\ -1.57 \end{pmatrix} \text{ (GeV)}. \quad (39)$$

This shows that the magnitude of ΔM_t is close to that of $\Delta\bar{m}_t(\bar{m}_t)$.

The final results for the top-quark OS mass are as follows:

$$M_t|_{\text{Conv.}} = 172.26_{-1.58}^{+2.29} \text{ (GeV)}, \quad (40)$$

$$M_t|_{\text{PMC}} = 172.41_{-1.57}^{+2.21} \text{ (GeV)}, \quad (41)$$

where the average uncertainties are squared with respect to those of $\Delta M_t|_{\text{High order}}$, $\Delta M_t|_{\Delta\alpha_s(M_Z)}$, and $\Delta M_t|_{\Delta\bar{m}_t(\bar{m}_t)}$, respectively. Among these uncertainties, the one caused by $\Delta\bar{m}_t(\bar{m}_t)$ is dominant¹⁾; more accurate data are needed to suppress this uncertainty.

We compare our results with experimental measurements [9, 75, 110] and some other theoretical predictions based on the analyses of top-pair production at hadronic colliders [46–48] in Table 1. All the predictions are consistent with each other within reasonable errors. Owing to the large input error of the top-quark $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$, our results show larger uncertainty than those of Refs. [46–48]. Up to the present known N⁴LO level, the predictions under the PMC and conventional scale-setting approaches are both consistent with the latest experimental measurements [9].

Table 1. A comparison of the top-quark OS mass M_t under various approaches. Refs. [46–48] derive the magnitude of the OS mass by comparing experimental data with theoretical predictions on the top-pair production cross-sections at hadronic colliders.

	M_t /GeV
PMC (this study)	$172.41_{-1.57}^{+2.21}$
Conv. (this study)	$172.26_{-1.58}^{+2.29}$
CMS [9]	172.93 ± 1.36
PDG [75]	172.5 ± 0.7
ATLAS and CMS [110]	$173.4_{-2.0}^{+1.8}$
[46]	172.5 ± 1.4
[47]	$171.54_{-0.31}^{+0.28}$
[48]	173.0 ± 0.6

At present, the experimentally measured value of top-quark OS mass is more precise than that of the top-quark $\overline{\text{MS}}$ mass. Thus, one can extract the $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$ by inversely using Eq. (23) or the resultant PMC series. This is discussed in the following section.

C. Extracting the top-quark $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$

Using experimental results of OS mass is also a suitable approach for extracting the $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$. The PDG [75] reports that the world average results of top-quark OS mass is $M_t = 172.5 \pm 0.7$ GeV, exhibiting a higher accuracy than that of the top-quark $\overline{\text{MS}}$ mass, i.e., $\bar{m}_t(\bar{m}_t) = 162.5_{-1.5}^{+2.1}$ GeV.

In the conventional scale-setting approach, one can extract the $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$ by using Eq. (23) and setting the renormalization scale $\mu_r = \bar{m}_t(\bar{m}_t)$:

$$\bar{m}_t(\bar{m}_t)|_{\text{Conv.}} = 162.73_{-0.67}^{+0.67} \text{ (GeV)}, \quad (42)$$

where the central value is obtained by setting $M_t = 172.5$ GeV and the uncertainty is caused by $\Delta M_t = \pm 0.7$ GeV.

Considering the uncertainty of the renormalization scale $\mu_r \in [\frac{1}{2}\bar{m}_t(\bar{m}_t), 2\bar{m}_t(\bar{m}_t)]$, we obtain

$$\bar{m}_t(\bar{m}_t)|_{\text{Conv.}} = 162.73_{-1.16}^{+0.00} \text{ (GeV)}, \quad (43)$$

Thus, the conventional prediction is

$$\bar{m}_t(\bar{m}_t)|_{\text{Conv.}} = 162.73_{-1.34}^{+0.67} \text{ (GeV)}, \quad (44)$$

where the average uncertainty is squared with respect to that of $\Delta M_t = \pm 0.7$ GeV and the renormalization scale

1) If the value of $\bar{m}_t(\bar{m}_t)$ can be measured very accurately to avoid the $\Delta\bar{m}_t(\bar{m}_t)$ uncertainty, we will obtain $M_t|_{\text{Conv.}} = 172.26_{-0.13}^{+0.64}$ (GeV), and $M_t|_{\text{PMC}} = 172.41_{-0.09}^{+0.11}$ (GeV).

$$\mu_r \in [\frac{1}{2}\bar{m}_t(\bar{m}_t), 2\bar{m}_t(\bar{m}_t)].$$

In the PMC scale-setting approach, one can extract the $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t)$ by using the PMC series without renormalization scale uncertainty:

$$M_t = \bar{m}_t(Q_*)\{1 + \hat{r}_{1,0}a_s(Q_*) + \hat{r}_{2,0}a_s^2(Q_*) + \hat{r}_{3,0}a_s^3(Q_*) + \hat{r}_{4,0}a_s^4(Q_*) + \text{O}[a_s^5(Q_*)]\}, \quad (45)$$

where the PMC scale Q_* satisfies Eq. (28). Thus, the PMC prediction is

$$\bar{m}_t(\bar{m}_t)|_{\text{PMC}} = 163.08^{+0.66}_{-0.66} \text{ (GeV)}, \quad (46)$$

where the central value is obtained by setting $M_t = 172.5$ GeV and the uncertainty is caused by $\Delta M_t = \pm 0.7$ GeV. It can be demonstrated that the PMC result predicted by Eq. (46) is more accurate than the conventional result predicted by Eq. (44). Finally, these results overlap with those of a previous study of ours, $\bar{m}_t(\bar{m}_t) = 162.6^{+0.4}_{-0.4}$ GeV, obtained by using the RGE of α_s alone [95] and the experimental result $\bar{m}_t(\bar{m}_t) = 162.9 \pm 0.5 \pm 1.0^{+2.1}_{-1.2}$ GeV [10].

IV. SUMMARY

In the present paper, we have derived new degeneracy relations with the help of the RGEs involving both the β -function and quark mass anomalous dimension γ_m -function, leading to improved PMC scale-setting procedures. Such procedures can be used to eliminate the conventional renormalization scale ambiguity of the fixed-order pQCD series under the $\overline{\text{MS}}$ running mass scheme, which simultaneously determines the correct magnitudes of α_s and the $\overline{\text{MS}}$ running mass \bar{m}_q of the perturbative series with the help of RGEs. By applying such formulas,

we have obtained a scale-invariant $\overline{\text{MS}}$ -on-shell quark mass relation. Consequently, we have determined the top-quark on-shell or $\overline{\text{MS}}$ mass without conventional renormalization scale ambiguity. By setting the top-quark $\overline{\text{MS}}$ mass as $\bar{m}_t(\bar{m}_t) = 162.5^{+2.1}_{-1.5}$ given in PDG as an input, we obtain the top-quark OS mass $M_t|_{\text{PMC}} = 172.41^{+2.21}_{-1.57}$ (GeV). It can be demonstrated that this result is characterized by a larger uncertainty than the experimental value, given that the input error $\Delta\bar{m}_t(\bar{m}_t)$ still exhibits a larger magnitude. We have also inversely determined the top-quark $\overline{\text{MS}}$ mass $\bar{m}_t(\bar{m}_t) = 163.08^{+0.66}_{-0.66}$ by using the top-quark OS mass $M_t = 172.5 \pm 0.7$ GeV as input; the resultant prediction of the top-quark $\overline{\text{MS}}$ mass is more precise than the experimental value given in PDG.

The accuracy of the pQCD prediction under the $\overline{\text{MS}}$ running mass scheme strongly depends on the exact values of α_s and \bar{m}_q . After applying the PMC, the correct values of the effective α_s and \bar{m}_q can be determined simultaneously, resulting in a more convergent pQCD series that leads to a much smaller residual scale dependence. Thus, a reliable and precise pQCD prediction can be achieved. This is also a useful method to determine the bottom-quark OS mass and charm-quark OS mass in the future.

ACKNOWLEDGMENTS

We thank Sheng-Quan Wang, Jian-Ming Shen, Jun Zeng and Qing Yu for helpful discussions.

APPENDIX A: SCALE DISPLACEMENT RELATIONS

The general scale displacement relations of the strong coupling constant a_s and quark running mass \bar{m}_q up to fourth-order are

$$a_s^k(\mu_r) = a_s^k(\mu_\delta) + k\beta_0\delta a_s^{k+1}(\mu_\delta) + k\left(\beta_1\delta + \frac{k+1}{2}\beta_0^2\delta^2\right)a_s^{k+2}(\mu_\delta)\delta + k\left[\beta_2 + \frac{2k+3}{2}\beta_0\beta_1\delta^2 + \frac{(k+1)(k+2)}{3!}\beta_0^3\delta^3\right]a_s^{k+3}(\mu_\delta) + \text{O}[a_s^{k+4}(\mu_\delta)]. \quad (A1)$$

$$\begin{aligned} \bar{m}_q^n(\mu_r) = \bar{m}_q^n(\mu_\delta) & \left\{ 1 + n\gamma_0\delta a_s + \left[\frac{1}{2}(n\beta_0\gamma_0 + n^2\gamma_0^2)\delta^2 + n\gamma_1\delta \right] a_s^2 + \left[n\gamma_2\delta + \frac{1}{2}(2n\beta_0\gamma_1 \right. \right. \\ & + n\beta_1\gamma_0 + 2n^2\gamma_0\gamma_1)\delta^2 + \frac{1}{3!}\left(2n\beta_0^2\gamma_0 + 3n^2\beta_0\gamma_0^2 + n^3\gamma_0^3 \right)\delta^3 \Big] a_s^3 + \left[n\gamma_3\delta \right. \\ & + \frac{1}{2}\left(3n\beta_0\gamma_2 + 2n\beta_1\gamma_1 + n\beta_2\gamma_0 + 2n^2\gamma_0\gamma_2 + n^2\gamma_1^2 \right)\delta^2 + \frac{1}{3!}\left(6n\beta_0^2\gamma_1 + 5n\beta_0\beta_1\gamma_0 \right. \\ & \left. \left. + 9n^2\beta_0\gamma_0\gamma_1 + 3n^2\beta_1\gamma_0^2 + 3n^3\gamma_0^2\gamma_1 \right)\delta^3 + \frac{1}{4!}\left(6n\beta_0^3\gamma_0 + 11n^2\beta_0^2\gamma_0^2 + 6n^3\beta_0\gamma_0^3 + n^4\gamma_0^4 \right)\delta^4 \right] a_s^4 + \text{O}(a_s^5) \Big\}. \quad (A2) \end{aligned}$$

APPENDIX B: EXPRESSION OF ρ_δ UP TO a_s^4 -ORDER

$$\begin{aligned}
\rho_\delta(Q^2) = & r_0 \bar{m}_q^n(\mu_\delta) \left\{ 1 + (r_1 + n\gamma_0\delta) a_s(\mu_\delta) + \left[r_2 + \beta_0 r_1 \delta + n(\gamma_1 + \gamma_0 r_1) \delta + \frac{n}{2} \beta_0 \gamma_0 \delta^2 + \frac{n^2}{2} \gamma_0^2 \delta^2 \right] a_s^2(\mu_\delta) \right. \\
& + \left[r_3 + \beta_1 r_1 \delta + 2\beta_0 r_2 \delta + \beta_0^2 r_1 \delta^2 + n(\gamma_2 + \gamma_0 r_2 + \gamma_1 r_1) \delta + n\beta_0 \left(\gamma_1 + \frac{3\gamma_0 r_1}{2} \right) \delta^2 + \frac{n}{2} \beta_1 \gamma_0 \delta^2 + \frac{n}{3} \beta_0^2 \gamma_0 \delta^3 \right. \\
& + n^2 \left(\gamma_1 \gamma_0 + \frac{\gamma_0^2 r_1}{2} \right) \delta^2 + \frac{n^2}{2} \beta_0 \gamma_0^2 \delta^3 + \frac{n^3}{6} \gamma_0^3 \delta^3 \left. \right] a_s^3(\mu_\delta) + \left[r_4 + (2\beta_1 r_2 + \beta_2 r_1) \delta + 3\beta_0 r_3 \delta + \frac{5}{2} \beta_0 \beta_1 r_1 \delta^2 + 3\beta_0^2 r_2 \delta^2 \right. \\
& + \beta_0^3 r_1 \delta^3 + n(\gamma_3 + \gamma_0 r_3 + \gamma_1 r_2 + \gamma_2 r_1) \delta + n\beta_0 \left(\frac{3\gamma_2}{2} + \frac{5\gamma_0 r_2}{2} + 2\gamma_1 r_1 \right) \delta^2 + n \left(\frac{\beta_2 \gamma_0}{2} + \beta_1 \gamma_1 + \frac{3}{2} \beta_1 \gamma_0 r_1 \right) \delta^2 \\
& + n\beta_0^2 \left(\gamma_1 + \frac{11\gamma_0 r_1}{6} \right) \delta^3 + \frac{5n}{6} \beta_0 \beta_1 \gamma_0 \delta^3 + \frac{n}{4} \beta_0^3 \gamma_0 \delta^4 + n^2 \left(\gamma_2 \gamma_0 + \frac{\gamma_1^2}{2} + \frac{\gamma_0^2 r_2}{2} + \gamma_1 \gamma_0 r_1 \right) \delta^2 + n^2 \beta_0 \left(\frac{3\gamma_1 \gamma_0}{2} + \gamma_0^2 r_1 \right) \delta^3 \\
& \left. + \frac{n^2}{2} \beta_1 \gamma_0^2 \delta^3 + \frac{11n^2}{24} \beta_0^2 \gamma_0^2 \delta^4 + n^3 \left(\frac{\gamma_1 \gamma_0^2}{2} + \frac{\gamma_0^3 r_1}{6} \right) \delta^3 + \frac{n^3}{4} \beta_0 \gamma_0^3 \delta^4 + \frac{n^4}{24} \gamma_0^4 \delta^4 \right] a_s^4(\mu_\delta) + \mathcal{O}[a_s^5(\mu_\delta)] \left. \right\}. \tag{B1}
\end{aligned}$$

APPENDIX C: EXPRESSION OF ρ UP TO a_s^4 -ORDER

$$\begin{aligned}
\rho(Q^2) = & r_0 \bar{m}_q^n(\mu_r) \left\{ 1 + \left(\hat{r}_{1,0} + n\gamma_0 \ln \frac{\mu_r^2}{Q^2} \right) a_s(\mu_r) + \left[\hat{r}_{2,0} + \beta_0 \hat{r}_{2,1} + n\gamma_0 \hat{r}_{2,1} + (\beta_0 \hat{r}_{1,0} + n\gamma_1 + n\gamma_0 \hat{r}_{1,0}) \ln \frac{\mu_r^2}{Q^2} \right. \right. \\
& + \frac{1}{2} (n\beta_0 \gamma_0 + n^2 \gamma_0^2) \ln^2 \frac{\mu_r^2}{Q^2} \left. \right] a_s^2(\mu_r) + \{ \hat{r}_{3,0} + \beta_1 \hat{r}_{2,1} + 2\beta_0 \hat{r}_{3,1} + \beta_0^2 \hat{r}_{3,2} + n(\gamma_0 \hat{r}_{3,1} + \gamma_1 \hat{r}_{2,1}) + \frac{3n}{2} \beta_0 \gamma_0 \hat{r}_{3,2} \\
& + \frac{n^2}{2} \gamma_0^2 \hat{r}_{3,2} + [\beta_1 \hat{r}_{1,0} + 2\beta_0 \hat{r}_{2,0} + 2\beta_0^2 \hat{r}_{2,1} + n(\gamma_2 + \gamma_1 \hat{r}_{1,0} + \gamma_0 \hat{r}_{2,0} + 3\beta_0 \gamma_0 \hat{r}_{2,1} + n\gamma_0^2 \hat{r}_{2,1})] \ln \frac{\mu_r^2}{Q^2} \\
& + \left[\beta_0^2 \hat{r}_{1,0} + n(\beta_0 \gamma_1 + \frac{1}{2} \beta_1 \gamma_0 + \frac{3}{2} \beta_0 \gamma_0 \hat{r}_{1,0}) + n^2 (\gamma_0 \gamma_1 + \frac{1}{2} \gamma_0^2 \hat{r}_{1,0}) \right] \ln^2 \frac{\mu_r^2}{Q^2} + \frac{1}{6} (2n\beta_0^2 \gamma_0 + 3n^2 \beta_0 \gamma_0^2 + n^3 \gamma_0^3) \ln^3 \frac{\mu_r^2}{Q^2} \left. \right\} a_s^3(\mu_r) \\
& + \left\{ \hat{r}_{4,0} + \beta_2 \hat{r}_{2,1} + 2\beta_1 \hat{r}_{3,1} + 3\beta_0 \hat{r}_{4,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{3,2} + 3\beta_0^2 \hat{r}_{4,2} + \beta_0^3 \hat{r}_{4,3} + n\beta_0 \left(2\gamma_1 \hat{r}_{3,2} + \frac{5}{2} \gamma_0 \hat{r}_{4,2} \right) \right. \\
& + n \left(\frac{3}{2} \beta_1 \gamma_0 \hat{r}_{3,2} + \gamma_2 \hat{r}_{2,1} + \gamma_1 \hat{r}_{3,1} + \gamma_0 \hat{r}_{4,1} \right) + \frac{11n}{6} \beta_0^2 \gamma_0 \hat{r}_{4,3} + n^2 \left(\frac{\gamma_0^2 \hat{r}_{4,2}}{2} + \gamma_1 \gamma_0 \hat{r}_{3,2} \right) + n^2 \beta_0 \gamma_0^2 \hat{r}_{4,3} + \frac{n^3}{6} \gamma_0^3 \hat{r}_{4,3} \\
& + \left[\beta_2 \hat{r}_{1,0} + 2\beta_1 \hat{r}_{2,0} + 3\beta_0 \hat{r}_{3,0} + 6\beta_0^2 \hat{r}_{3,1} + 3\beta_0^3 \hat{r}_{3,2} + 5\beta_1 \beta_0 \hat{r}_{2,1} + n \left(\gamma_3 + \gamma_2 \hat{r}_{1,0} + \gamma_1 \hat{r}_{2,0} + \gamma_0 \hat{r}_{3,0} + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{3,2} \right. \right. \\
& + 4\beta_0 \gamma_1 \hat{r}_{2,1} + 5\beta_0 \gamma_0 \hat{r}_{3,1} + 3\beta_1 \gamma_0 \hat{r}_{2,1} \left. \right) + n^2 (3\beta_0 \gamma_0^2 \hat{r}_{3,2} + 2\gamma_0 \gamma_1 \hat{r}_{2,1}) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{3,2} \left. \right] \ln \frac{\mu_r^2}{Q^2} \\
& + \left[3\beta_0^2 \hat{r}_{2,0} + 3\beta_0^3 \hat{r}_{2,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{1,0} + n \left(\frac{3}{2} \beta_0 \gamma_2 + \beta_1 \gamma_1 + \frac{1}{2} \beta_2 \gamma_0 + \frac{3}{2} \beta_1 \gamma_0 \hat{r}_{1,0} + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{2,1} + 2\beta_0 \gamma_1 \hat{r}_{1,0} + \frac{5}{2} \beta_0 \gamma_0 \hat{r}_{2,0} \right) \right. \\
& + n^2 \left(\frac{1}{2} \gamma_1^2 + \gamma_0 \gamma_2 + \gamma_0 \gamma_1 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \hat{r}_{2,0} + 3\beta_0 \gamma_0^2 \hat{r}_{2,1} \right) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{2,1} \left. \right] \ln^2 \frac{\mu_r^2}{Q^2} + \left[\beta_0^3 \hat{r}_{1,0} + n \left(\beta_0^2 \gamma_1 + \frac{11}{6} \beta_0^2 \gamma_0 \hat{r}_{1,0} + \frac{5}{6} \beta_0 \beta_1 \gamma_0 \right) \right. \\
& + n^2 \left(\beta_0 \gamma_0^2 \hat{r}_{1,0} + \frac{1}{2} \beta_1 \gamma_0^2 + \frac{3}{2} \beta_0 \gamma_0 \gamma_1 \right) + n^3 \left(\frac{1}{6} \gamma_0^3 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \gamma_1 \right) \left. \right] \ln^3 \frac{\mu_r^2}{Q^2} \\
& \left. + \left(\frac{n}{4} \beta_0^3 \gamma_0 + \frac{11n^2}{24} \beta_0^2 \gamma_0^2 + \frac{n^3}{4} \beta_0 \gamma_0^3 + \frac{n^4}{24} \gamma_0^4 \right) \ln^4 \frac{\mu_r^2}{Q^2} \right\} a_s^4(\mu_r) + \mathcal{O}[a_s^5(\mu_r)] \left. \right\}. \tag{C1}
\end{aligned}$$

APPENDIX D: RELATIONSHIPS BETWEEN $r_k(\mu_r^2/Q^2)$ ($k = 3, 4$) AND $\hat{r}_{i,j}$

$$r_3(\mu_r^2/Q^2) = \hat{r}_{3,0} + \beta_1 \hat{r}_{2,1} + 2\beta_0 \hat{r}_{3,1} + \beta_0^2 \hat{r}_{3,2} + n(\gamma_0 \hat{r}_{3,1} + \gamma_1 \hat{r}_{2,1}) + \frac{3n}{2} \beta_0 \gamma_0 \hat{r}_{3,2} + \frac{n^2}{2} \gamma_0^2 \hat{r}_{3,2} + [\beta_1 \hat{r}_{1,0} + 2\beta_0 \hat{r}_{2,0} + 2\beta_0^2 \hat{r}_{2,1}$$

$$\begin{aligned}
& + n(\gamma_2 + \gamma_1 \hat{r}_{1,0} + \gamma_0 \hat{r}_{2,0} + 3\beta_0 \gamma_0 \hat{r}_{2,1} + n\gamma_0^2 \hat{r}_{2,1}) \ln \frac{\mu_r^2}{Q^2} + [\beta_0^2 \hat{r}_{1,0} + n(\beta_0 \gamma_1 + \frac{1}{2} \beta_1 \gamma_0 + \frac{3}{2} \beta_0 \gamma_0 \hat{r}_{1,0}) \\
& + n^2(\gamma_0 \gamma_1 + \frac{1}{2} \gamma_0^2 \hat{r}_{1,0})] \ln^2 \frac{\mu_r^2}{Q^2} + \frac{1}{6} (2n\beta_0^2 \gamma_0 + 3n^2 \beta_0 \gamma_0^2 + n^3 \gamma_0^3) \ln^3 \frac{\mu_r^2}{Q^2},
\end{aligned} \tag{D1}$$

$$\begin{aligned}
r_4(\mu_r^2/Q^2) = & \hat{r}_{4,0} + \beta_2 \hat{r}_{2,1} + 2\beta_1 \hat{r}_{3,1} + 3\beta_0 \hat{r}_{4,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{3,2} + 3\beta_0^2 \hat{r}_{4,2} + \beta_0^3 \hat{r}_{4,3} + n\beta_0 (2\gamma_1 \hat{r}_{3,2} + \frac{5}{2} \gamma_0 \hat{r}_{4,2}) \\
& + n \left(\frac{3}{2} \beta_1 \gamma_0 \hat{r}_{3,2} + \gamma_2 \hat{r}_{2,1} + \gamma_1 \hat{r}_{3,1} + \gamma_0 \hat{r}_{4,1} \right) + \frac{11n}{6} \beta_0^2 \gamma_0 \hat{r}_{4,3} + n^2 \left(\frac{\gamma_0^2 \hat{r}_{4,2}}{2} + \gamma_1 \gamma_0 \hat{r}_{3,2} \right) + n^2 \beta_0 \gamma_0^2 \hat{r}_{4,3} + \frac{n^3}{6} \gamma_0^3 \hat{r}_{4,3} \\
& + \left[\beta_2 \hat{r}_{1,0} + 2\beta_1 \hat{r}_{2,0} + 3\beta_0 \hat{r}_{3,0} + 6\beta_0^2 \hat{r}_{3,1} + 3\beta_0^3 \hat{r}_{3,2} + 5\beta_1 \beta_0 \hat{r}_{2,1} + n \left(\gamma_3 + \gamma_2 \hat{r}_{1,0} + \gamma_1 \hat{r}_{2,0} + \gamma_0 \hat{r}_{3,0} \right. \right. \\
& + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{3,2} + 4\beta_0 \gamma_1 \hat{r}_{2,1} + 5\beta_0 \gamma_0 \hat{r}_{3,1} + 3\beta_1 \gamma_0 \hat{r}_{2,1} \left. \left. + n^2 (3\beta_0 \gamma_0^2 \hat{r}_{3,2} + 2\gamma_0 \gamma_1 \hat{r}_{2,1}) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{3,2} \right] \ln \frac{\mu_r^2}{Q^2} \\
& + \left[3\beta_0^2 \hat{r}_{2,0} + 3\beta_0^3 \hat{r}_{2,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{1,0} + n \left(\frac{3}{2} \beta_0 \gamma_2 + \beta_1 \gamma_1 + \frac{1}{2} \beta_2 \gamma_0 + \frac{3}{2} \beta_1 \gamma_0 \hat{r}_{1,0} + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{2,1} + 2\beta_0 \gamma_1 \hat{r}_{1,0} + \frac{5}{2} \beta_0 \gamma_0 \hat{r}_{2,0} \right) \right. \\
& + n^2 \left(\frac{1}{2} \gamma_1^2 + \gamma_0 \gamma_2 + \gamma_0 \gamma_1 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \hat{r}_{2,0} + 3\beta_0 \gamma_0^2 \hat{r}_{2,1} \right) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{2,1} \left. \right] \ln^2 \frac{\mu_r^2}{Q^2} + \left[\beta_0^3 \hat{r}_{1,0} + n \left(\beta_0^2 \gamma_1 + \frac{11}{6} \beta_0^2 \gamma_0 \hat{r}_{1,0} \right. \right. \\
& + \frac{5}{6} \beta_0 \beta_1 \gamma_0 \left. \left. + n^2 \left(\beta_0 \gamma_0^2 \hat{r}_{1,0} + \frac{1}{2} \beta_1 \gamma_0^2 + \frac{3}{2} \beta_0 \gamma_0 \gamma_1 \right) + n^3 \left(\frac{1}{6} \gamma_0^3 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \gamma_1 \right) \right] \ln^3 \frac{\mu_r^2}{Q^2} \\
& + \left(\frac{n}{4} \beta_0^3 \gamma_0 + \frac{11n^2}{24} \beta_0^2 \gamma_0^2 + \frac{n^3}{4} \beta_0 \gamma_0^3 + \frac{n^4}{24} \gamma_0^4 \right) \ln^4 \frac{\mu_r^2}{Q^2}.
\end{aligned} \tag{D2}$$

APPENDIX E: DEGENERACY RELATION

It is possible to infer some degenerate relations from Eq. (B1). For example, the coefficients of $\beta_0 a_s^2$, $n\gamma_0 a_s^2$, $\beta_1 a_s^3$, $n\gamma_1 a_s^3$, $\beta_2 a_s^4$, and $n\gamma_2 a_s^4$ are the same, namely $r_{1,\delta}$. By substituting $r_i \delta^j \rightarrow r_{i+j,j}$, the expression for ρ at $\mu_r = Q$ can be rewritten as

$$\begin{aligned}
\rho(Q^2) = & r_0 \bar{m}_q^n(Q) \left\{ 1 + \hat{r}_{1,0} a_s(Q) + (\hat{r}_{2,0} + \beta_0 \hat{r}_{2,1} + n\gamma_0 \hat{r}_{2,1}) a_s^2(Q) + \left[\hat{r}_{3,0} + \beta_1 \hat{r}_{2,1} + 2\beta_0 \hat{r}_{3,1} + \beta_0^2 \hat{r}_{3,2} + n(\gamma_0 \hat{r}_{3,1} + \gamma_1 \hat{r}_{2,1}) + \frac{3n}{2} \beta_0 \gamma_0 \hat{r}_{3,2} \right. \right. \\
& + \frac{n^2}{2} \gamma_0^2 \hat{r}_{3,2} \left. \right] a_s^3(Q) + \left[\hat{r}_{4,0} + \beta_2 \hat{r}_{2,1} + 2\beta_1 \hat{r}_{3,1} + 3\beta_0 \hat{r}_{4,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{3,2} + 3\beta_0^2 \hat{r}_{4,2} + \beta_0^3 \hat{r}_{4,3} + n\beta_0 \left(2\gamma_1 \hat{r}_{3,2} + \frac{5}{2} \gamma_0 \hat{r}_{4,2} \right) \right. \\
& + n \left(\frac{3}{2} \beta_1 \gamma_0 \hat{r}_{3,2} + \gamma_2 \hat{r}_{2,1} + \gamma_1 \hat{r}_{3,1} + \gamma_0 \hat{r}_{4,1} \right) + \frac{11n}{6} \beta_0^2 \gamma_0 \hat{r}_{4,3} + n^2 \left(\frac{\gamma_0^2 \hat{r}_{4,2}}{2} + \gamma_1 \gamma_0 \hat{r}_{3,2} \right) \\
& \left. \left. + n^2 \beta_0 \gamma_0^2 \hat{r}_{4,3} + \frac{n^3}{6} \gamma_0^3 \hat{r}_{4,3} \right] a_s^4(Q) + \mathcal{O}[a_s^5(Q)] \right\}.
\end{aligned} \tag{E1}$$

A pQCD calculation prediction for a physical observable at $\mu_r = Q$ is

$$\rho(Q^2) = r_0 \bar{m}_q^n(Q) \left[1 + \sum_{k=1}^{\infty} \left(\sum_{l=0}^{k-1} c_{k,l} n_f^l \right) a_s^k(Q) \right]. \tag{E2}$$

Comparing Eq. (E1) with Eq. (E2) for each order, the coefficients of the n_f series can be matched to the $r_{i,j}$ coefficients in a unique manner. More explicitly, one can derive the relations between $c_{k,l}$ and $r_{i,j}$ by using the β_i and γ_i coefficients given in [70, 72]; e.g., it is easy to find that $\hat{r}_{1,0} = c_{1,0}$. Substituting $\beta_0 = 11 - \frac{2}{3} n_f$ and $\gamma_0 = 4$ into the a_s^2 -order coefficient of Eq. (E1), we can find $r_{2,0}$ and $r_{2,1}$:

$$c_{2,0} + c_{2,1}n_f = \hat{r}_{2,0} + \left(11 - \frac{2}{3}n_f\right)\hat{r}_{2,1} + 4n\hat{r}_{2,1}, \quad (\text{E3})$$

which leads to

$$\hat{r}_{1,0} = c_{1,0}, \quad (\text{E4})$$

$$\hat{r}_{2,0} = c_{2,0} + \left(6n + \frac{33}{2}\right)c_{2,1}, \quad \hat{r}_{2,1} = -\frac{3}{2}c_{2,1}. \quad (\text{E5})$$

Following the same procedures, one can derive these relations up to any order. In the present paper, we use the relations up to fourth order:

$$\begin{aligned} \hat{r}_{3,0} &= c_{3,0} + \left(3n + \frac{33}{2}\right)c_{3,1} + \left(9n^2 + 99n + \frac{1089}{4}\right)c_{3,2} - \left(10n^2 + 11n + \frac{321}{2}\right)c_{2,1}, \\ \hat{r}_{3,1} &= -\frac{3}{4}c_{3,1} - \frac{27n+99}{4}c_{3,2} + \frac{10n+57}{4}c_{2,1}, \quad \hat{r}_{3,2} = \frac{9}{4}c_{3,2}, \end{aligned} \quad (\text{E6})$$

$$\begin{aligned} \hat{r}_{4,0} &= c_{4,0} + \left(2n + \frac{33}{2}\right)c_{4,1} + \left(4n^2 + 66n + \frac{1089}{4}\right)c_{4,2} + \left(8n^3 + 198n^2 + \frac{3267n}{2} + \frac{35937}{8}\right)c_{4,3} \\ &\quad - \left(\frac{50n^3}{3} + 185n^2 + \frac{2595n}{2} + \frac{10593}{2}\right)c_{3,2} - \left(\frac{10n^2}{3} + 15n + \frac{321}{2}\right)c_{3,1} \\ &\quad + \left(\frac{20n^3}{27} - 160\zeta_3n^2 - \frac{2411n^2}{9} - \frac{860n}{3} - 1320\zeta_3n + \frac{11675}{16}\right)c_{2,1}, \end{aligned} \quad (\text{E7})$$

$$\begin{aligned} \hat{r}_{4,1} &= -\frac{1}{2}c_{4,1} - \frac{1}{2}(5n+33)c_{4,2} - \left(\frac{19n^2}{2} + \frac{495n}{4} + \frac{3267}{8}\right)c_{4,3} + \left(\frac{5n}{6} + \frac{19}{2}\right)c_{3,1} + \left(\frac{85n^2}{6} + \frac{401n}{4} + \frac{4113}{8}\right)c_{3,2} \\ &\quad + \left(\frac{100n^2}{27} + 40\zeta_3n + \frac{2467n}{72} - \frac{479}{4}\right)c_{2,1}, \end{aligned} \quad (\text{E8})$$

$$\hat{r}_{4,2} = \frac{3}{4}c_{4,2} + \left(\frac{33n}{4} + \frac{297}{8}\right)c_{4,3} - \left(5n + \frac{285}{8}\right)c_{3,2} + \left(\frac{325}{48} - \frac{35n}{18}\right)c_{2,1}, \quad (\text{E9})$$

$$\hat{r}_{4,3} = -\frac{27}{8}c_{4,3}. \quad (\text{E10})$$

Note that one must treat the n_f terms which are not related to renormalization of the running coupling and running mass as part of the conformal coefficient; e.g., the n_f terms coming from the light-by-light diagrams in QCD belong to the conformal series. The contributions of light-by-light diagrams are always established separately, given that the light-by-light diagrams can be easily distinguished from the other Feynman diagrams.

APPENDIX F: $r_{i,\text{NonConf.}}(i = 3, 4)$

$$r_{3,\text{NonConf.}}(Q^*) = \beta_1\hat{r}_{2,1} + 2\beta_0\hat{r}_{3,1} + \beta_0^2\hat{r}_{3,2} + n(\gamma_0\hat{r}_{3,1} + \gamma_1\hat{r}_{2,1}) + \frac{3n}{2}\beta_0\gamma_0\hat{r}_{3,2} + \frac{n^2}{2}\gamma_0^2\hat{r}_{3,2} + \left[\beta_1\hat{r}_{1,0} + 2\beta_0\hat{r}_{2,0} + 2\beta_0^2\hat{r}_{2,1}\right]$$

$$\begin{aligned}
 & + n(\gamma_2 + \gamma_1 \hat{r}_{1,0} + \gamma_0 \hat{r}_{2,0} + 3\beta_0 \gamma_0 \hat{r}_{2,1} + n\gamma_0^2 \hat{r}_{2,1}) \ln \frac{Q_*^2}{Q^2} + \left[\beta_0^2 \hat{r}_{1,0} + n(\beta_0 \gamma_1 + \frac{1}{2} \beta_1 \gamma_0 + \frac{3}{2} \beta_0 \gamma_0 \hat{r}_{1,0}) \right. \\
 & \left. + n^2(\gamma_0 \gamma_1 + \frac{1}{2} \gamma_0^2 \hat{r}_{1,0}) \right] \ln^2 \frac{Q_*^2}{Q^2} + \frac{1}{6} (2n\beta_0^2 \gamma_0 + 3n^2 \beta_0 \gamma_0^2 + n^3 \gamma_0^3) \ln^3 \frac{Q_*^2}{Q^2}, \tag{F1}
 \end{aligned}$$

$$\begin{aligned}
 r_{4,\text{NonConf.}}(Q_*) & = \beta_2 \hat{r}_{2,1} + 2\beta_1 \hat{r}_{3,1} + 3\beta_0 \hat{r}_{4,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{3,2} + 3\beta_0^2 \hat{r}_{4,2} + \beta_0^3 \hat{r}_{4,3} + n\beta_0 (2\gamma_1 \hat{r}_{3,2} + \frac{5}{2} \gamma_0 \hat{r}_{4,2}) \\
 & + n \left(\frac{3}{2} \beta_1 \gamma_0 \hat{r}_{3,2} + \gamma_2 \hat{r}_{2,1} + \gamma_1 \hat{r}_{3,1} + \gamma_0 \hat{r}_{4,1} \right) + \frac{11n}{6} \beta_0^2 \gamma_0 \hat{r}_{4,3} + n^2 \left(\frac{\gamma_0^2 \hat{r}_{4,2}}{2} + \gamma_1 \gamma_0 \hat{r}_{3,2} \right) + n^2 \beta_0 \gamma_0^2 \hat{r}_{4,3} \\
 & + \frac{n^3}{6} \gamma_0^3 \hat{r}_{4,3} + \left[\beta_2 \hat{r}_{1,0} + 2\beta_1 \hat{r}_{2,0} + 3\beta_0 \hat{r}_{3,0} + 6\beta_0^2 \hat{r}_{3,1} + 3\beta_0^3 \hat{r}_{3,2} + 5\beta_1 \beta_0 \hat{r}_{2,1} + n(\gamma_3 + \gamma_2 \hat{r}_{1,0} + \gamma_1 \hat{r}_{2,0}) \right. \\
 & \left. + \gamma_0 \hat{r}_{3,0} + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{3,2} + 4\beta_0 \gamma_1 \hat{r}_{2,1} + 5\beta_0 \gamma_0 \hat{r}_{3,1} + 3\beta_1 \gamma_0 \hat{r}_{2,1} \right] + n^2 (3\beta_0 \gamma_0^2 \hat{r}_{3,2} + 2\gamma_0 \gamma_1 \hat{r}_{2,1}) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{3,2} \ln \frac{Q_*^2}{Q^2} \\
 & + \left[3\beta_0^2 \hat{r}_{2,0} + 3\beta_0^3 \hat{r}_{2,1} + \frac{5}{2} \beta_0 \beta_1 \hat{r}_{1,0} + n \left(\frac{3}{2} \beta_0 \gamma_2 + \beta_1 \gamma_1 + \frac{1}{2} \beta_2 \gamma_0 + \frac{3}{2} \beta_1 \gamma_0 \hat{r}_{1,0} + \frac{11}{2} \beta_0^2 \gamma_0 \hat{r}_{2,1} + 2\beta_0 \gamma_1 \hat{r}_{1,0} + \frac{5}{2} \beta_0 \gamma_0 \hat{r}_{2,0} \right) \right. \\
 & \left. + n^2 \left(\frac{1}{2} \gamma_1^2 + \gamma_0 \gamma_2 + \gamma_0 \gamma_1 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \hat{r}_{2,0} + 3\beta_0 \gamma_0^2 \hat{r}_{2,1} \right) + \frac{n^3}{2} \gamma_0^3 \hat{r}_{2,1} \right] \ln^2 \frac{Q_*^2}{Q^2} \\
 & + \left[\beta_0^3 \hat{r}_{1,0} + n(\beta_0^2 \gamma_1 + \frac{11}{6} \beta_0^2 \gamma_0 \hat{r}_{1,0} + \frac{5}{6} \beta_0 \beta_1 \gamma_0) + n^2 (\beta_0 \gamma_0^2 \hat{r}_{1,0} + \frac{1}{2} \beta_1 \gamma_0^2 + \frac{3}{2} \beta_0 \gamma_0 \gamma_1) \right. \\
 & \left. + n^3 \left(\frac{1}{6} \gamma_0^3 \hat{r}_{1,0} + \frac{1}{2} \gamma_0^2 \gamma_1 \right) \right] \ln^3 \frac{Q_*^2}{Q^2} + \left(\frac{n}{4} \beta_0^3 \gamma_0 + \frac{11n^2}{24} \beta_0^2 \gamma_0^2 + \frac{n^3}{4} \beta_0 \gamma_0^3 + \frac{n^4}{24} \gamma_0^4 \right) \ln^4 \frac{Q_*^2}{Q^2}. \tag{F2}
 \end{aligned}$$

APPENDIX G: S_3

$$\begin{aligned}
 S_3 & = \hat{r}_{1,0} \hat{r}_{3,1} - \hat{r}_{1,0}^2 \hat{r}_{2,1} + \hat{r}_{2,0} \hat{r}_{2,1} - \hat{r}_{4,1} + \frac{n\gamma_0}{2} (\hat{r}_{2,1}^2 + \hat{r}_{1,0} \hat{r}_{3,2} - \hat{r}_{4,2}) - \frac{n\gamma_1 \hat{r}_{3,2}}{2} - \frac{n^2 \gamma_0^2 \hat{r}_{4,3}}{6} - \frac{\beta_2 \hat{r}_{2,1}}{n\gamma_0} \\
 & + \beta_1 \left(\frac{\gamma_1 \hat{r}_{2,1}}{n\gamma_0^2} + \frac{2\hat{r}_{1,0} \hat{r}_{2,1} - 2\hat{r}_{3,1}}{n\gamma_0} - \frac{3\hat{r}_{3,2}}{2} \right) + \beta_0 \beta_1 \left(\frac{2\hat{r}_{1,0} \hat{r}_{2,1}}{n^2 \gamma_0^2} - \frac{5\hat{r}_{3,2}}{2n\gamma_0} \right) + \beta_0 \left(\frac{5\hat{r}_{2,1}^2}{2} - n\gamma_0 \hat{r}_{4,3} - \frac{5\hat{r}_{4,2}}{2} + 2\hat{r}_{1,0} \hat{r}_{3,2} - \frac{\gamma_1^2 \hat{r}_{2,1}}{n\gamma_0^3} \right. \\
 & \left. + \frac{\gamma_2 \hat{r}_{2,1} + 2\gamma_1 \hat{r}_{3,1} - 2\gamma_1 \hat{r}_{1,0} \hat{r}_{2,1}}{n\gamma_0^2} - \frac{n\gamma_1 \hat{r}_{3,2} + 6\hat{r}_{2,1} \hat{r}_{1,0}^2 - 6\hat{r}_{3,1} \hat{r}_{1,0} - 6\hat{r}_{2,0} \hat{r}_{2,1} + 6\hat{r}_{4,1}}{2n\gamma_0} \right) + \beta_0^2 \left(\frac{7\hat{r}_{2,1}^2 + 5\hat{r}_{1,0} \hat{r}_{3,2} - 6\hat{r}_{4,2}}{2n\gamma_0} \right. \\
 & \left. + \frac{n\gamma_1 \hat{r}_{3,2} - 3\hat{r}_{2,1} \hat{r}_{1,0}^2 + 2\hat{r}_{3,1} \hat{r}_{1,0} + 2\hat{r}_{2,0} \hat{r}_{2,1}}{n^2 \gamma_0^2} - \frac{2\gamma_1 \hat{r}_{1,0} \hat{r}_{2,1}}{n^3 \gamma_0^3} - \frac{11\hat{r}_{4,3}}{6} \right) + \beta_0^3 \left(\frac{3\hat{r}_{2,1}^2 + 2\hat{r}_{1,0} \hat{r}_{3,2}}{2n^2 \gamma_0^2} - \frac{\hat{r}_{2,1} \hat{r}_{1,0}^2}{n^3 \gamma_0^3} - \frac{\hat{r}_{4,3}}{n\gamma_0} \right). \tag{G1}
 \end{aligned}$$

References

- | | |
|---|---|
| [1] M. Aaboud, <i>et al.</i> (ATLAS), <i>Phys. Lett. B</i> 761 , 350 (2016) | [8] A. Tumasyan <i>et al.</i> (CMS), <i>JHEP</i> 12 , 161 (2021) |
| [2] M. Aaboud <i>et al.</i> (ATLAS), <i>JHEP</i> 09 , 118 (2017) | [9] A. Tumasyan <i>et al.</i> (CMS), <i>JHEP</i> 07 , 077 (2023) |
| [3] M. Aaboud <i>et al.</i> (ATLAS), <i>Eur. Phys. J. C</i> 79 , 290 (2019) | [10] G. Aad <i>et al.</i> (ATLAS), <i>JHEP</i> 11 , 150 (2019) |
| [4] V. Khachatryan <i>et al.</i> (CMS), <i>Phys. Rev. D</i> 93 , 072004 (2016) | [11] A. M. Sirunyan <i>et al.</i> (CMS), <i>Eur. Phys. J. C</i> 80 , 658 (2020) |
| [5] A. M. Sirunyan <i>et al.</i> (CMS), <i>Phys. Rev. D</i> 96 , 032002 (2017) | [12] M. Aaboud <i>et al.</i> (ATLAS), <i>Eur. Phys. J. C</i> 77 , 804 (2017) |
| [6] A. M. Sirunyan <i>et al.</i> (CMS), <i>Eur. Phys. J. C</i> 78 , 891 (2018) | [13] G. Aad <i>et al.</i> (ATLAS), <i>JHEP</i> 10 , 121 (2015) |
| [7] A. M. Sirunyan <i>et al.</i> (CMS), <i>Eur. Phys. J. C</i> 79 , 313 (2019) | [14] A. M. Sirunyan <i>et al.</i> (CMS), <i>Phys. Rev. Lett.</i> 124 , 202001 (2020) |
| | [15] A. M. Sirunyan <i>et al.</i> (CMS), <i>Eur. Phys. J. C</i> 77 , 354 (2017) |

- [16] V. M. Abazov *et al.* (D0), *Phys. Rev. D* **94**, 092004 (2016)
- [17] V. M. Abazov *et al.* (D0), *Phys. Lett. B* **703**, 422 (2011)
- [18] A. Buckley *et al.*, *Phys. Rep.* **504**, 145 (2011)
- [19] P. Z. Skands and D. Wick, *Eur. Phys. J. C* **52**, 133 (2007)
- [20] S. Kawabata, Y. Shimizu, Y. Sumino *et al.*, *Phys. Lett. B* **741**, 232 (2015)
- [21] J. Kieseler, K. Lipka, and S. O. Moch, *Phys. Rev. Lett.* **116**, 162001 (2016)
- [22] B. Dehnadi, A. H. Hoang, V. Mateu *et al.*, *Proc. Sci. RADCOR2017*, 062 (2018)
- [23] A. H. Hoang, *Ann. Rev. Nucl. Part. Sci.* **70**, 225 (2020)
- [24] S. Fleming, A. H. Hoang, S. Mantry *et al.*, *Phys. Rev. D* **77**, 074010 (2008)
- [25] V. Khachatryan *et al.* (CMS), *J. High Energy Phys.* **08**, 029 (2016)
- [26] S. Ferrario Ravasio, T. Ježo, P. Nason, and C. Oleari, *Eur. Phys. J. C* **78**, 458 (2018)
- [27] M. Butenschoen, B. Dehnadi, A. H. Hoang *et al.*, *Phys. Rev. Lett.* **117**, 232001 (2016)
- [28] (ATLAS, CDF, CMS and D0), *First combination of Tevatron and LHC measurements of the top-quark mass*, arXiv: 1403.4427 [hep-ex]
- [29] S. Moch, S. Weinzierl, S. Alekhin *et al.* *High precision fundamental constants at the TeV scale*, arXiv: 1405.4781 [hep-ph]
- [30] A. Juste, S. Mantry, A. Mitov *et al.*, *Eur. Phys. J. C* **74**, 3119 (2014)
- [31] A. H. Hoang, *The Top Mass: Interpretation and Theoretical Uncertainties*, arXiv: 1412.3649 [hep-ph]
- [32] A. M. Sirunyan *et al.* (CMS), *Eur. Phys. J. C* **79**, 368 (2019)
- [33] R. Hempfling and B. A. Kniehl, *Phys. Rev. D* **51**, 1386 (1995)
- [34] K. G. Chetyrkin and M. Steinhauser, *Phys. Rev. Lett.* **83**, 4001 (1999)
- [35] F. Jegerlehner and M. Y. Kalmykov, *Nucl. Phys.* **B676**, 365 (2004)
- [36] S. P. Martin, *Phys. Rev. D* **72**, 096008 (2005)
- [37] A. B. Galtieri, F. Margaroli, and I. Volobouev, *Rept. Prog. Phys.* **75**, 056201 (2012)
- [38] S. P. Martin, *Phys. Rev. D* **93**, 094017 (2016)
- [39] P. Nason, *Proc. Sci. TOP2015*, 056 (2016)
- [40] M. Beneke, P. Marquard, P. Nason *et al.*, *Phys. Lett. B* **775**, 63 (2017)
- [41] G. Bevilacqua, H. B. Hartanto, M. Kraus *et al.*, *JHEP* **03**, 169 (2018)
- [42] S. Q. Wang, X. G. Wu, Z. G. Si *et al.*, *Eur. Phys. J. C* **78**, 237 (2018)
- [43] P. Marquard, A. V. Smirnov, V. A. Smirnov *et al.*, *PoS RADCOR2017*, 029 (2018)
- [44] C. Ayala, X. Lobregat, and A. Pineda, *Phys. Rev. D* **101**, 034002 (2020)
- [45] W. L. Ju, G. Wang, X. Wang *et al.*, *JHEP* **06**, 158 (2020)
- [46] S. Q. Wang, X. G. Wu, J. M. Shen *et al.*, *Chin. Phys. C* **45**, 113102 (2021)
- [47] M. V. Garzelli, J. Mazzitelli, S. O. Moch *et al.*, *Top-quark pole mass extraction at NNLO accuracy, from total, single- and double-differential cross sections for $t\bar{t} + X$ production at the LHC*, arXiv: 2311.05509 [hep-ph]
- [48] T. Cridge and M. A. Lim, *Eur. Phys. J. C* **83**, 805 (2023)
- [49] A. M. Cooper-Sarkar, M. Czakon, M. A. Lim *et al.*, *Simultaneous extraction of α_s and m_t from LHC $t\bar{t}$ differential distributions*, arXiv: 2010.04171 [hep-ph]
- [50] M. S. Gao, S. R. Yuan, and J. Gao, *JHEP* **04**, 054 (2021)
- [51] M. Beneke, *Eur. Phys. J. ST* **230**, 2565 (2021)
- [52] S. Alioli, J. Fuster, M. V. Garzelli *et al.*, *Top-quark mass extraction from $t\bar{t}j + X$ events at the LHC: theory predictions*, arXiv: 2203.07344 [hep-ph]
- [53] R. Tarrach, *Nucl. Phys.* **B183**, 384 (1981)
- [54] N. Gray, D. J. Broadhurst, W. Grafe *et al.*, *Z. Phys. C* **48**, 673 (1990)
- [55] K. G. Chetyrkin and M. Steinhauser, *Nucl. Phys. B* **573**, 617 (2000)
- [56] K. Melnikov and T. V. Ritbergen, *Phys. Lett. B* **482**, 99 (2000)
- [57] F. Jegerlehner, M. Y. Kalmykov, and O. Veretin, *Nucl. Phys.* **B658**, 49 (2003)
- [58] F. Jegerlehner and M. Y. Kalmykov, *Acta Phys. Polon. B* **34**, 5335 (2003)
- [59] M. Faisst, J. H. Kuhn, and O. Veretin, *Phys. Lett. B* **589**, 35 (2004)
- [60] P. Marquard, L. Mihaila, J. H. Piclum *et al.*, *Nucl. Phys. B* **773**, 1 (2007)
- [61] P. Marquard, A. V. Smirnov, V. A. Smirnov *et al.*, *Phys. Rev. Lett.* **114**, 142002 (2015)
- [62] P. Marquard, A. V. Smirnov, V. A. Smirnov *et al.*, *Phys. Rev. D* **94**, 074025 (2016)
- [63] A. L. Kataev and V. S. Molokoedov, *JETP Lett.* **108**, 777 (2018)
- [64] A. L. Kataev and V. S. Molokoedov, *Theor. Math. Phys.* **200**, 1374 (2019)
- [65] A. L. Kataev and V. S. Molokoedov, *Eur. Phys. J. C* **80**, 1160 (2020)
- [66] H. D. Politzer, *Phys. Rev. Lett.* **30**, 1346 (1973)
- [67] D. J. Gross and F. Wilczek, *Phys. Rev. Lett.* **30**, 1343 (1973)
- [68] H. D. Politzer, *Phys. Rep.* **14**, 129 (1974)
- [69] D. J. Gross and F. Wilczek, *Phys. Rev. D* **8**, 3633 (1973)
- [70] P. A. Baikov, K. G. Chetyrkin *et al.*, *Phys. Rev. Lett.* **118**, 082002 (2017)
- [71] K. G. Chetyrkin, *Nucl. Phys.* **B710**, 499 (2005)
- [72] P. A. Baikov, K. G. Chetyrkin *et al.*, *JHEP* **10**, 076 (2014)
- [73] J. A. M. Vermaseren, S. A. Larin, and T. van Ritbergen, *Phys. Lett. B* **405**, 327 (1997)
- [74] K. G. Chetyrkin, *Phys. Lett. B* **404**, 161 (1997)
- [75] R.L. Workman *et al.* (Particle Data Group), *PTEP* **2022**, 083C01 (2022)
- [76] S. J. Brodsky and X. G. Wu, *Phys. Rev. D* **85**, 034038 (2012)
- [77] S. J. Brodsky and L. Di Giustino, *Phys. Rev. D* **86**, 085026 (2012)
- [78] S. J. Brodsky and X. G. Wu, *Phys. Rev. Lett.* **109**, 042002 (2012)
- [79] M. Mojaza, S. J. Brodsky, and X. G. Wu, *Phys. Rev. Lett.* **110**, 192001 (2013)
- [80] S. J. Brodsky, G. P. Lepage, and P. B. Mackenzie, *Phys. Rev. D* **28**, 228 (1983)
- [81] S. J. Brodsky, L. Di Giustino, P. G. Ratcliffe *et al.*, *Phys. Lett. B* **847**, 138288 (2023), arXiv:2311.17360 [hep-ph]
- [82] P. M. Stevenson, *Phys. Lett. B* **100**, 61 (1981)
- [83] P. M. Stevenson, *Phys. Rev. D* **23**, 2916 (1981)
- [84] X. G. Wu, Y. Ma, S. Q. Wang *et al.*, *Rept. Prog. Phys.* **78**, 126201 (2015)
- [85] Y. Ma, X. G. Wu, H. H. Ma *et al.*, *Phys. Rev. D* **91**, 034006 (2015)
- [86] Y. Ma and X. G. Wu, *Phys. Rev. D* **97**, 036024 (2018)

- [87] S. J. Brodsky and X. G. Wu, *Phys. Rev. D* **86**, 054018 (2012)
- [88] X. G. Wu, S. J. Brodsky, and M. Mojaza, *Prog. Part. Nucl. Phys.* **72**, 44 (2013)
- [89] X. G. Wu, J. M. Shen, B. L. Du *et al.*, *Phys. Rev. D* **97**, 094030 (2018)
- [90] X. G. Wu, J. M. Shen, B. L. Du *et al.*, *Prog. Part. Nucl. Phys.* **108**, 103706 (2019)
- [91] L. Di Giustino, S. J. Brodsky, P. G. Ratcliffe *et al.*, *High precision tests of QCD without scale or scheme ambiguities*, arXiv: 2307.03951 [hep-ph]
- [92] B. L. Du, X. G. Wu, J. M. Shen *et al.*, *Eur. Phys. J. C* **79**, 182 (2019)
- [93] Q. Yu, X. G. Wu, J. Zeng *et al.*, *Eur. Phys. J. C* **80**, 362 (2020)
- [94] Q. Yu, X. G. Wu, S. Q. Wang *et al.*, *Chin. Phys. C* **43**, 093102 (2019)
- [95] X. D. Huang, X. G. Wu, J. Zeng *et al.*, *Phys. Rev. D* **101**, 114024 (2020)
- [96] H. M. Yu, W. L. Sang, X. D. Huang *et al.*, *JHEP* **01**, 131 (2021)
- [97] X. D. Huang, X. G. Wu, X. C. Zheng *et al.*, *Eur. Phys. J. C* **81**, 291 (2021)
- [98] X. D. Huang, X. G. Wu, Q. Yu *et al.*, *Nucl. Phys. B* **969**, 115466 (2021)
- [99] S. J. Brodsky, M. Mojaza, and X. G. Wu, *Phys. Rev. D* **89**, 014027 (2014)
- [100] J. M. Shen, X. G. Wu, B. L. Du *et al.*, *Phys. Rev. D* **95**, 094006 (2017)
- [101] D. Salinas-Arizmendi and I. Schmidt, *Relation between polar and running masses of heavy quarks using the principle of maximum conformality*, arXiv: 2209.06881 [hep-ph]
- [102] S. Q. Wang, X. G. Wu, X. C. Zheng *et al.*, *Eur. Phys. J. C* **74**, 2825 (2014)
- [103] H. Y. Bi, X. G. Wu, Y. Ma *et al.*, *Phys. Lett. B* **748**, 13 (2015)
- [104] F. Herren and M. Steinhauser, *Comput. Phys. Commun.* **224**, 333 (2018)
- [105] X. C. Zheng, X. G. Wu, S. Q. Wang *et al.*, *J. High Energy Phys.* **10**, 117 (2013)
- [106] J. L. Basdevant, *Fortsch. Phys.* **20**, 283 (1972)
- [107] M. A. Samuel, G. Li, and E. Steinfelds, *Phys. Lett. B* **323**, 188 (1994)
- [108] M. A. Samuel, J. R. Ellis, and M. Karliner, *Phys. Rev. Lett.* **74**, 4380 (1995)
- [109] E. Gardi, *Phys. Rev. D* **56**, 68 (1997)
- [110] G. Aad *et al.* (ATLAS and CMS), *JHEP* **07**, 213 (2023)