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Generalization of the Brodsky-Lepage-Mackenzie optimization within the $\{\beta\}$-expansion and the principle of maximal conformality

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We discuss generalizations of the Brodsky–Lepage–Mackenzie optimization procedure for renormalization group invariant quantities. In this respect, we discuss in detail the features and construction of the $\{\beta\}$-expansion presentation instead of the standard perturbative series with regard to the Adler D function and Bjorken polarized sum rules obtained in the order of $\mathcal{O}(\alpha_s^4)$. Based on the $\{\beta\}$ expansion, we analyze different schemes of optimization, including the corrected principle of maximal conformality, numerically illustrating their results. We suggest our scheme for the series optimization and apply it to both the above quantities.

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I. INTRODUCTION

The problem of scale-scheme dependence ambiguities in the renormalization-group (RG) calculations [1] remains important. In the past few years, a new extension of the Brodsky–Lepage–Mackenzie (BLM) scale-fixing approach [2], called the principle of maximal conformality (PMC), was started [3] and formulated in more detail in Refs. [4–7] with a variety of applications to phenomenologically oriented studies.

Here, we show that the PMC approach is closely related to the sequential BLM (seBLM) method, originally proposed in Ref. [8] for the analysis of the next-to-next-to-leading-order (NNLO) QCD prediction for quantities like the e^+e^--annihilation R ratio. This method was based on the RG-inspired presentation of the $\{\beta\}$ expansion for perturbative series, the one later used for other purposes in Refs. [9,10]. The seBLM was constructed as a generalization of the works devoted to the extension of the BLM $\overline{\rm MS}$-type scale-fixing prescription to the level of NNLO QCD corrections [11,12] and beyond [13–16].

In this paper, we will use the $\{\beta\}$-expansion presentation and the seBLM method to study the e^+e^--annihilation R ratio, the related Adler function $D^{\rm EM}$ of the electromagnetic quark currents, and the Bjorken sum rule $S^{\rm Bjp}$ of the polarized lepton-nucleon deep-inelastic scattering (DIS). We will clarify the concrete theoretical shortcomings of the PMC QCD studies performed in a number of works on the subject, in particular, in Refs. [4–7], and will present the results for the corrected PMC approach.

Certain problems of the misuse of the PMC approach to the Adler function were already emphasized in Ref. [17] but not recognized in the recently published work [7]. We will clarify these theoretical problems in more detail and consider the existing modification of the NNLO PMC analysis, based on application of the seBLM method, which allows one to reproduce the original next-to-leading-order (NLO) BLM expression from the considerations performed in Ref. [7] and already discussed in Ref. [17]. Note that the necessity of introducing modifications to the analysis of Ref. [7] starts to manifest itself from the level of taking into account the second-order perturbative corrections to the R ratio evaluated analytically in Ref. [18] in the minimal subtractions (MS) scheme proposed in Ref. [19]. This result was also obtained numerically in Ref. [20] and confirmed analytically in Ref. [21] by using the $\overline{\rm MS}$ scheme of Ref. [22]. At the level of the third-order corrections to $D^{\rm EM}$, analytically calculated in the $\overline{\rm MS}$ scheme [23,24] and confirmed in the independent work [25], there appear additional differences between the results of the PMC and the seBLM methods.

We present several arguments in favor of theoretical and phenomenological applications of the form of the β-expanded expressions for the RG invariant (RGI) quantities proposed in Ref. [8] and applied in Ref. [9].[1] In this respect, let us mention the QCD generalization (in the $\overline{\rm MS}$ scheme) of the Crewther relation [27] based on the $\{\beta\}$ expansion [9]. Using the results of these relations, we obtain in a self-consistent way the NNLO $\{\beta\}$ expansion for $S^{\rm Bjp}(Q^2)$ in QCD with $n_{\tilde{g}}$ numbers of gluinos, which can be checked by direct analytical calculations.

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[1]Note that the $\{\beta\}$-expansion representation is related in part to the expansion of the perturbative terms, considered in Ref. [26], in the RGI Green functions through the powers of the first coefficient of the β function.

The article is organized as follows. In Sec. II, we define single-scale RG invariant quantities for the e^+e^- annihilation to hadrons and for the DIS inclusive processes, which will be studied in this work. The existing theoretical relations between perturbative expressions for these characteristics are also summarized. In Sec. III, the $\{\beta\}$ expansion of the RGI quantities, proposed in Ref. [8] and applied in Refs. [9,10], is revisited and discussed in detail. Using the results of Ref. [8] and the "multiple power β-function" QCD expression [9] for the $\overline{\rm MS}$-scheme generalization of the Crewther relation [27], we provide the arguments that this expansion is unique. The details of constructing the $\{\beta\}$ expansions for the Adler $D^{\rm EM}$ function and for the $S^{\rm Bjp}$ sum rule are described at the level of the $O(a_s^3)$ corrections, where $a_s = \alpha_s/(4\pi)$. In Sec. IV A, we consider the relations between certain terms of the $\{\beta\}$ expansion for $D^{\rm EM}$ and $S^{\rm Bjp}$, which will be obtained from the Crewther relation of Ref. [27] and its QCD generalization of Ref. [9], and present the concrete $\{\beta\}$-expanded contributions to the $D^{\rm EM}$ function, R ratio, and the $S^{\rm Bjp}$ sum rule.

Using our definition of the $\{\beta\}$-expansion representation, we correct the values of the PMC coefficients and the scales in the related powers of the PMC perturbative expressions for the Adler function $D^{\rm EM}$ and $R_{e^+e^-}$ ratio, presented in Refs. [4–7], and discuss their correspondence to the results obtained in Refs. [8,9,17]. The discussion of the results of the BLM, seBLM, and PMC procedures together with the numerical estimates of the corresponding perturbation theory (PT) coefficients and the couplings at new normalization scales are presented in Sec. V. It is demonstrated that, in spite of its theoretical prominence following from the conformal symmetry relations, even the corrected PMC procedure does not improve the convergence of perturbative series for the R ratio and for the $S^{\rm Bjp}$ sum rule. The methods of further optimizations of these series, which are based on the $\{\beta\}$ expansion, are elaborated on in Sec. VI. The technical results are presented in the Appendixes.

II. DEFINITIONS OF THE BASIC QUANTITIES

Consider first the Adler function $D^{\rm EM}(Q^2)$, which is expressed through the two-point correlator of the electromagnetic vector currents $j_\mu^{\rm EM} = \sum_i q_i \bar{\psi}_i \gamma_\mu \psi_i$ taken at Euclidean $-q^2 = Q^2$. Here, q_i stands for the electric charge of the quark field ψ_i. $D^{\rm EM}(Q^2)$ consists of the sum of its nonsinglet (NS) and singlet (S) parts

$$D^{\rm EM}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right) = \left(\sum_i q_i^2\right) d_R D^{\rm NS}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right) + \left(\sum\nolimits_i q_i\right)^2 d_R D^{\rm S}\left(\frac{Q^2}{\mu^2}, a_s(\mu^2)\right), \tag{2.1a}$$

where

$$D^{\rm NS}(Q^2/\mu^2, a_s(\mu^2)) = 1 + \sum_{l\geq 1} d_l^{\rm NS}(Q^2/\mu^2) a_s^l(\mu^2), \tag{2.1b}$$

$$D^{\rm S}(Q^2/\mu^2, a_s(\mu^2)) = \frac{d^{abc}d^{abc}}{d_R} \sum_{l\geq 3} d_l^{\rm S}(Q^2/\mu^2) a_s^l(\mu^2). \tag{2.1c}$$

Here, d_R is the dimension of the Lie algebra related to the $SU(N_c)$ group (in the fundamental representation $d_R = N_c$), and $d^{abc} = 2{\rm Tr}(\{\lambda^a/2, \lambda^b/2\}, \lambda^c/2)$ is the symmetric tensor. Both the NS and S contributions to the Adler function are the RGI quantities calculable in the Euclidean domain. After applying the RG equation, they can be represented as

$$D^{\rm NS}(Q^2/\mu^2, a_s(\mu^2)) \stackrel{\mu^2=Q^2}{\longrightarrow} D^{\rm NS}(a_s(Q^2)) = 1 + \sum_{l\geq 1} d_l^{\rm NS} a_s^l(Q^2) \tag{2.2a}$$

$$D^{\rm S}(Q^2/\mu^2, a_s(\mu^2)) \stackrel{\mu^2=Q^2}{\longrightarrow} D^{\rm S}(a_s(Q^2)) = \frac{d^{abc}d^{abc}}{d_R} \sum_{l\geq 3} d_l^{\rm S} a_s^l(Q^2). \tag{2.2b}$$

Because of the cancellation of the logarithms $\ln^k(Q^2/\mu^2)$ with $k \geq l+1$ in the terms $d_l^a(Q^2/\mu^2)$ (the superscript a defines the contributions to the NS and S parts of the $D^{\rm EM}$-function), the coefficients of $d_l^a \equiv d_l^a(1)$ are the numbers in the MS-like schemes.

Let us emphasize that in this work we use the perturbative expansion parameter $a_s(\mu^2)$ normalized as $a_s(\mu^2) \equiv \alpha_s(\mu^2)/4\pi$. It obeys the RG equation with the consistently normalized $SU(N_c)$-group β function

$$\mu^2 \frac{{\rm d}}{{\rm d}\mu^2} a_s(\mu) = \beta(a_s) = -a_s^2 \sum_{i\geq 0} \beta_i a_s^i, \tag{2.3}$$

where $\beta_0 = (11/3 C_{\rm A} - (4/3) T_{\rm R} n_f)$, while other coefficients β_i are presented in Appendix A.

The quantity related to the observable total cross section of the $e^+e \to$ hadrons process $R_{e^+e^-}(s) = \sigma(e^+e^- \to {\rm hadrons})/\sigma(e^+e^- \to \mu^+\mu^-)$ is measured in the Minkowski region $(s > 0)$; this can be obtained from the $D^{\rm EM}$ function as

$$R_{e^+e^-}(s) \equiv R(s, \mu^2 = s) = \frac{1}{2\pi i}\int_{-s-i\varepsilon}^{-s+i\varepsilon} \frac{D^{\rm EM}(\sigma/\mu^2; a_s(\mu^2))}{\sigma} d\sigma\bigg|_{\mu^2=s}$$
$$= \left(\sum_i q_i^2\right) d_R\left(1 + \sum_{m\geq 1} r_m^{\rm NS} a_s^m(s)\right) + \left(\sum\nolimits_i q_i\right)^2 \frac{d^{abc}d^{abc}}{d_R}\sum_{n\geq 3} r_n^{\rm S} a_s^n(s). \quad (2.4)$$

The coefficients r_m^a for the a part (a = NS or S) of $R_{e^+e^-}$ are associated with the coefficients d_l^a of the D^a function by the triangular matrix T^a of the relation $r_m^a = T_{ml}^a d_l^a$, which will be discussed in Sec. IV C and Table I.

The next observable RGI quantity we will be interested in is the Bjorken polarized sum rule $S^{\rm Bjp}$. It is defined by the integral over the difference of the spin-dependent structure functions of the polarized lepton-proton and lepton-neutron deep-inelastic scattering as

$$S^{\rm Bjp}(Q^2) = \int_0^1 [g_1^{lp}(x,Q^2) - g_1^{ln}(x,Q^2)]dx$$
$$= \frac{g_A}{6} C^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)), \quad (2.5)$$

where g_A is the nucleon axial charge as measured in the neutron β decay and $C^{\rm Bjp}(a_s)$ is the coefficient function calculable within perturbation theory and not damped by the inverse powers of Q^2, i.e., the leading-twist term.

The application of the operator-product expansion (OPE) method in the MS-like scheme [28] and the knowledge on the perturbative structure of the $\overline{\rm MS}$-scheme QCD generalization of the quark-parton model Crewther relation [27] gained from articles in Refs. [29–35] indicate the existence of the previously undiscussed singlet contribution to $C^{\rm Bjp}(a_s)$ [36]. Using the results of this work, we define the overall perturbative expression for $C^{\rm Bjp}$ as

$$C^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) = C_{\rm NS}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) + \left(\sum_i q_i\right) C_{\rm S}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)), \quad (2.6)$$

where the NS and S coefficient functions can be written down as

$$C_{\rm NS}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) = 1 + \sum_{l\geq 1} c_l^{\rm NS}(Q^2/\mu^2) a_s^l(\mu^2) \quad (2.7)$$

$$C_{\rm S}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) = \frac{d^{abc}d^{abc}}{d_R}\sum_{l\geq 3} c_l^{\rm S}(Q^2/\mu^2) a_s^l(\mu^2) \quad (2.8)$$

and have the following RG-improved form:

$$C_{\rm NS}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) \overset{\mu^2=Q^2}{\longrightarrow} C_{\rm NS}^{\rm Bjp}(a_s(Q^2)) = 1 + \sum_{l\geq 1} c_l^{\rm NS} a_s^l(Q^2), \quad (2.9a)$$

$$C_{\rm S}^{\rm Bjp}(Q^2/\mu^2, a_s(\mu^2)) \overset{\mu^2=Q^2}{\longrightarrow} C_{\rm S}^{\rm Bjp}(a_s(Q^2)) = \frac{d^{abc}d^{abc}}{d_R}\sum_{l\geq 3} c_l^{\rm S} a_s^{l+1}(Q^2), \quad (2.9b)$$

$$C^{\rm Bjp}(a_s(Q^2)) = C_{\rm NS}^{\rm Bjp}(a_s(Q^2)) + C_{\rm S}^{\rm Bjp}(a_s(Q^2)). \quad (2.9c)$$

The analytical expressions for the NLO and NNLO corrections to Eq. (2.9a) in the $\overline{\rm MS}$ scheme were evaluated in Refs. [37] and [38], respectively, while the corresponding next-to-next-to-next-to-leading-order (N^{3}LO) $\mathcal{O}(a_s^4)$ correction was calculated in Ref. [33] (its direct analytical form was also presented in Ref. [9]). The symbolic expression for the coefficient c_4^S of the $\mathcal{O}(a_s^4)$ correction to the singlet contribution $C_{\rm S}^{\rm Bjp}(a_s)$ of the Bjorken polarized sum rule was fixed in Ref. [36] from the $\overline{\rm MS}$-scheme generalization of the Crewther relation, which will be presented below.

Let us also consider the Gross–Llewellyn -Smith (GLS) sum rule of the deep-inelastic neutrino-nucleon scattering. Its leading-twist perturbative QCD expression can be defined as

$$S_{\rm GLS}(Q^2) = \frac{1}{2}\int_0^1 [F_3^{\nu p}(x,Q^2) + F_3^{\nu n}(x,Q^2)]dx$$
$$= 3C_{\rm GLS}(Q^2/\mu^2, a_s(\mu^2)), \quad (2.10)$$

where $F_3(x,Q^2)$ is the structure functions of the deep-inelastic neutrino-nucleon scattering process. The coefficient function on the rhs of Eq. (2.10) also contains both NS and S contributions, namely,

$$C_{\rm GLS}(Q^2/\mu^2, a_s(\mu^2)) = C_{\rm GLS}^{\rm NS}(Q^2/\mu^2, a_s(\mu^2)) + C_{\rm GLS}^{\rm S}(Q^2/\mu^2, a_s(\mu^2)). \quad (2.11)$$

As a consequence of the chiral invariance, which can be restored in the dimensional regularization [39] by means of additional finite renormalizations (for their evaluation in high-loop orders, see, e.g., Refs. [37,38,40,41]), the NS contributions to the leading-twist coefficient function of $S_{\rm GLS}(Q^2)$ coincide with a similar NS perturbative contribution $S^{\rm Bjp}(Q^2)$, namely,

$$\begin{aligned} C^{\rm NS}_{\rm GLS}(Q^2/\mu^2, a_s(\mu^2)) &\equiv C^{\rm Bjp}_{\rm NS}(Q^2/\mu^2, a_s(\mu^2)) \\ &= 1 + \sum_{l\geq 1} c^{\rm NS}_l (Q^2/\mu^2) a^l_s(\mu^2) \\ &\xrightarrow{\mu^2=Q^2} C^{\rm Bjp}_{\rm NS}(a_s(Q^2)) \\ &= 1 + \sum_{l\geq 1} c^{\rm NS}_l a^l_s(Q^2). \end{aligned} \tag{2.12}$$

The fulfilment of this identity was explicitly demonstrated in the existing analytical NLO and NNLO calculations in Refs. [37,38] and used as the input in the process of determination of the analytical expression for the $\mathcal{O}(a_s^4)$ corrections to $S_{\rm GLS}(Q^2)$ [34].

The second (singlet-type) contribution to the coefficient function of Eq. (2.11) has the form

$$\begin{aligned} C^{\rm S}_{\rm GLS}(Q^2/\mu^2, a_s(\mu^2)) &= n_f \frac{d^{abc}d^{abc}}{d_R} \sum_{l\geq 3} \bar{c}_l (Q^2/\mu^2) a^l_s(\mu^2) \\ &\xrightarrow{\mu^2=Q^2} C^{\rm S}_{\rm GLS}(a_s(Q^2)) \\ &= n_f \frac{d^{abc}d^{abc}}{d_R} \sum_{l\geq 3} \bar{c}_l\, a^l_s(Q^2), \end{aligned} \tag{2.13}$$

where $\bar{c}_3$ and $\bar{c}_4$ were evaluated analytically in Refs. [38] and [34], respectively.

The application of the OPE approach to the three-point functions of axial-vector-vector currents (see Refs. [30–32,35,36]) leads to the following $\overline{\rm MS}$-scheme QCD generalization of the Crewther relation (CR) between the different coefficient functions of the annihilation and deep-inelastic scattering processes introduced above,

$$C^{\rm Bjp}(a_s)D^{\rm NS}(a_s) \equiv C_{\rm GLS}(a_s)[D^{\rm NS}(a_s) + n_f D^{\rm S}(a_s)] \tag{2.14a}$$

$$= \mathbb{1} + \frac{\beta(a_s)}{a_s} \cdot P(a_s), \tag{2.14b}$$

where $\mathbb{1}$ was derived in Ref. [27] using the conformal symmetry, $\beta(a_s)$ is the RG β function, $a_s = a_s(Q^2)$, and the polynomial P is

$$P(a_s) = a_s K_1 + a_s^2 K_2 + a_s^3 K_3 + O(a_s^4). \tag{2.15}$$

It contains the coefficients K_1 and K_2, obtained in Ref. [29], while the analytical expression for the coefficient $K_3 = K_3^{\rm NS} + K_3^{\rm S}$ is the sum of the NS and S terms, which are given in Refs. [33] and [34], respectively. Note that Eq. (2.14a) was first published in Ref. [35] without taking into account singlet-type contributions to $C^{\rm Bjp}$. Their more careful analysis of Ref. [36] fixes the β_0-dependent analytical expression of the $\mathcal{O}(a_s^4)$ contribution to $C^{\rm Bjp}_{\rm S}$.[2]

The result of Ref. [36] and the general Eq. (2.14a) is not yet confirmed by direct analytical calculations. In our further studies we will use the product of their NS parts and the related to this product results of the expansion in Eq. (2.14b), reformulated in Ref. [9].

III. GENERAL β-EXPANSION STRUCTURE OF OBSERVABLES

A. Formulation of the approach

To clarify the main ideas of the $\{\beta\}$-expansion representation proposed in Ref. [8] for the perturbative coefficients of the RGI quantities, let us consider the NS part of the Adler function. Its expression can be rewritten as $D^{\rm NS} = 1 + d_1^{\rm NS} \cdot \sum_{n\geq 1} d_l a_s^l$, where $d_1^{\rm NS} = 3C_{\rm F}$ is the overall normalization factor. Within the $\{\beta\}$-expansion approach, the coefficients d_n, originally fixed in the $\overline{\rm MS}$ scheme, are expressed as

$$d_1 = d_1[0] = 1, \tag{3.1a}$$

$$d_2 = \beta_0 d_2[1] + d_2[0], \tag{3.1b}$$

$$d_3 = \beta_0^2 d_3[2] + \beta_1 d_3[0,1] + \beta_0 d_3[1] + d_3[0], \tag{3.1c}$$

$$\begin{aligned} d_4 = {}& \beta_0^3 d_4[3] + \beta_1\beta_0 d_4[1,1] + \beta_2 d_4[0,0,1] \\ & + \beta_0^2 d_4[2] + \beta_1 d_4[0,1] + \beta_0 d_4[1] \\ & d_4[0], \end{aligned} \tag{3.1d}$$

$$\vdots$$

$$d_N = \beta_0^{N-1} d_N[N-1] + \cdots + d_N[0], \tag{3.1e}$$

where the first argument of the expansion elements $d_n[n_0, n_1, \ldots]$ indicates its multiplication to the n_0th power of the first coefficient β_0 of the RG β function, namely, to the $\beta_0^{n_0}$ term. The second argument n_1 determines the power of the second multiplication factor, namely, $\beta_1^{n_1}$, and so on. The elements $d_n[0] \equiv d_n[0,0,\ldots,0]$ define "refined" β_i-independent corrections with powers $n_i = 0$ of all their $\beta_i^{n_i}$ multipliers. These elements coincide with expressions for the coefficients d_n in the imaginary situation of the nullified QCD β function in all orders of perturbation theory. This case corresponds to the effective restoration of the conformal symmetry limit of the bare $SU(N_c)$ model in the case in which all normalizations are not considered. This limit, extensively discussed in Ref. [17], will be considered here as a technical trick. The origins of other

[2] In QED the validity of Eq. (2.14a) follows from the considerations of Ref. [42].

elements in expansions in (3.1a)–(3.1e) were considered in Ref. [8].

The first elements $d_i[i-1]$ of the expansions of Eqs. (3.1b)–(3.1e) arise from the diagrams with a maximum number of the "fermion one-loop bubble" insertions and applications of the naive non-Abelization (NNA) approximation [43]). In the case of the $D^{\rm NS}$ function, they can be obtained from the result in Ref. [29], which follow from renormalon-type calculations in Refs. [44,45].

It should be stressed that the terms $\beta_0 d_3[1]$ in Eq. (3.1c) and $\beta_1 d_4[0,1]$, $\beta_0 d_4[1]$ in Eq. (3.1d) were not taken into account in the variant of the $\{\beta\}$-expansion method used in Refs. [4–6]. The omitting of these terms leads to the results, which should be corrected by including these terms in the self-consistent variant of the PMC analysis.

In high order of perturbation theory, one should also consider a similar expression of the singlet part $D^{\rm S} = d_3^{\rm S} \cdot \sum_{j\geq 3} \bar{d}_j a_s^{(j)}$ with the normalization factor $d_3^{\rm S} = 11/3 - 8\zeta_3$ evaluated first in the QED work [46] and the related normalizations of the defined coefficients in Eq. (2.13), namely, $\bar{d}_j = d_j^{\rm S}/d_3^{\rm S}$. The $\{\beta\}$-expanded coefficients of this RGI quantity are expressed as

$$\bar{d}_3 = \bar{d}_3[0] = 1 \tag{3.2a}$$

$$\bar{d}_4 = \beta_0 \bar{d}_4[1] + \bar{d}_4[0], \tag{3.2b}$$

$$\vdots$$

$$\bar{d}_{j+2} = \beta_0^{j-1} \bar{d}_{j+2}[j-1] + \cdots + \bar{d}_{j+2}[0]. \tag{3.2c}$$

The same ordering in the β-function coefficients can be applied to the coefficients c_n for the NS coefficient function of the deep-inelastic sum rules $C^{\rm NS}$ of Eq. (2.12) and to the singlet contribution $C^{\rm S}$ to the GLS sum rule [see Eq. (2.13)]. Moreover, it is possible to show that the elements of the corresponding $\{\beta\}$ expansions $d_n[n_0, n_1, \ldots]$ and $c_n[n_0, n_1, \ldots]$ are closely related [9]. We will return to a more detailed discussion of this property a bit later.

The above $\{\beta\}$ expansion can be interpreted as a "matrix" representation for the RGI quantities: For the quantity $D^{\rm NS}$ expanded up to an order of N, $D^{\rm NS} = \sum_{n=1}^N a_s^n \sum_{i\geq 0} D_{ni}^{\rm NS} B^{(i)}$, which is related to the traditional "vector" representation, $D^{\rm NS} = \sum_{n=1}^N a_s^n d_n$ with $d_n = \sum_i D_{ni}^{\rm NS} B^{(i)}$. Here, $B^{(i)}$ are the elements that express the structure of $\{\beta\}$-expanded perturbative coefficients and are convolved with the matrix elements $D_{ni}^{\rm NS} = d_n[\ldots]$. In the case of consideration of the refined β_i-independent corrections, $d_n[0] \equiv D_{n0}$ and $B^{(0)} = 1$. The similar matrix representation can be written down for the singlet part $D^{\rm S}$ with the $\{\beta\}$-expanded coefficient defined in Eqs. (3.2a)–(3.2c).

Note that the matrix representation contains new dynamical information about the RGI quantities, which is not contained in the vector one. Thus, Eqs. (3.1b) and (3.2b) can be considered as the initial points to apply the standard BLM procedure. The generalization of the BLM procedure to higher orders can be constructed using the $\{\beta\}$ expansions of higher-order coefficients of Eqs. (3.1c)–(3.1e) [8]. However, starting with the NNLO, the explicit solution of this problem is nontrivial.

B. Explicit determination of the structures of the $\{\beta\}$-expanded series for $D^{\rm NS}$

Let us start the discussion of application of the $\{\beta\}$-expansion procedure in the NLO. Imagine that we deal with the perturbative quenched QCD (pqQCD) approximation for the $D^{\rm NS}$ function in the NLO. It is described by the contributions of the three-loop photon vacuum polarization diagrams with closed external loop, formed by a quark-antiquark pair and connected by internal gluon propagators, which do not contain any internal quark-loop insertions. In this theoretical approximation, the coefficient d_2 takes the following form:

$$d_2 \to d_2^{\rm pqQCD} = -\frac{\rm C_F}{2} + \left(\frac{123}{2} - 44\zeta_3\right)\frac{\rm C_A}{3} \quad \text{with} \qquad \beta_0 = \frac{11}{3} C_{\rm A}. \tag{3.3}$$

In this case, it is unclear how to perform the standard BLM scale-fixing prescription in the NLO approximation. Indeed, it is not clear what is the expression for the $d_2[1]$ coefficient of the β_0 term of Eq. (3.1b) in the expression for $d_2^{\rm pqQCD}$. To obtain explicitly the elements of the expansion (3.1b) and extract the β_0 term in (3.3), one should take into account the quark-antiquark one-loop insertion in internal gluon lines of the three-loop approximation for the hadronic vacuum polarization function. This is equivalent to taking into account in the pqQCD model of the interacting with gluons of internal quark loops with $\boldsymbol{n_f}$ number of active quarks. The corresponding parameter $\boldsymbol{n_f}$ can be considered as a *mark* of the charge renormalization by the quark-antiquark pairs. It enters into both d_2 and β_0 expressions and allows one to extract *unambiguously* the expression for d_2 proportional to the β_0 term in the $\overline{\rm MS}$ scheme. Indeed, fixing $T_R = T_F = \frac{1}{2}$, we obtain

$$d_2 = -\frac{\rm C_F}{2} + \left(\frac{11\cdot 11 + 2}{2} - 44\zeta_3\right)\frac{\rm C_A}{3} - \left(\frac{11}{2} - 4\zeta_3\right)\frac{2}{3}\boldsymbol{n_f} \quad \text{with} \qquad \beta_0 = \frac{11}{3} C_{\rm A} - \frac{2}{3}\boldsymbol{n_f}. \tag{3.4}$$

To get the appropriate expression of the coefficient d_2, one should take into account the one-loop renormalization of charge. As a result, we immediately obtain from Eq. (3.4) the expression for the coefficient of Eq. (3.1b),

$$d_2 = \frac{\mathrm{C_A}}{3} - \frac{\mathrm{C_F}}{2} + \left(\frac{11}{2} - 4\zeta_3\right)\left(\frac{11}{3}\mathrm{C_A} - \frac{2}{3}\boldsymbol{n_f}\right), \quad (3.5a)$$

where

$$d_2[0] = \frac{\mathrm{C_A}}{3} - \frac{\mathrm{C_F}}{2}, \qquad d_2[1] = \frac{11}{2} - 4\zeta_3. \quad (3.5b)$$

This decomposition corresponds to the case of the standard BLM consideration in the $\overline{\mathrm{MS}}$ scheme [2]. Note that for $\boldsymbol{n_f} = 0$ this decomposition remains valid for the case of pqQCD (QCD at $\boldsymbol{n_f} = 0$) and leads to Eq. (3.5b).

Any additional modifications of QCD, say, by means of introducing into considerations $\boldsymbol{n_{\tilde g}}$ multiplets of a strong interacting gluino [the element of the minimal supersymmetric standard model (MSSM) model], will change in the NLO expression for the considered RGI quantity the content of the β_0 coefficient in the expression for d_2, calculated in the $\overline{\mathrm{MS}}$ scheme, but not the refined element and the coefficients at β_0 of Eq. (3.3). Using the result β_0 for the β function with the $\boldsymbol{n_{\tilde g}}$ multiplet of the strong interacting gluino [see Eq. (A1a)] and the D^{NS} function in the same model [presented in Eq. (A5b)], the same result (3.5b) for decomposition can unambiguously be obtained using the additional to $\boldsymbol{n_f}$ marks in Eq. (3.5a), namely, the number of strong-interacting gluinos $\boldsymbol{n_{\tilde g}}$. Indeed, combining the result

$$d_2 = \frac{\mathrm{C_A}}{3} - \frac{\mathrm{C_F}}{2} + \left(\frac{11}{2} - 4\zeta_3\right)\left(\frac{11}{3}\mathrm{C_A} - \frac{2}{3}\boldsymbol{n_f}\right) - (11 - 8\zeta_3)\boldsymbol{n_{\tilde g}}\frac{C_A}{3}, \quad (3.6a)$$

with

$$\beta_0(\boldsymbol{n_f}, \boldsymbol{n_{\tilde g}}) = \frac{11}{3}C_A - \frac{2}{3}(\boldsymbol{n_f} + \boldsymbol{n_{\tilde g}}C_A), \quad (3.6b)$$

we get the expressions for $d_2[0]$ and $d_2[1]$, which are identical to the ones presented in Eq. (3.5b). Note that these results can be obtained from Eqs. (3.6a) and (3.6b) with gluino degrees of freedom only ($\boldsymbol{n_{\tilde g}} \neq 0$, $\boldsymbol{n_f} = 0$) or only with the quark ones ($\boldsymbol{n_f} \neq 0$, $\boldsymbol{n_{\tilde g}} = 0$) or with taking into account both of them. The reason of this unambiguity is that the interaction of any new particle accumulated here in the charge renormalization is determined by the universal gauge group $SU(N_c)$.

All these possibilities give us a simple tool to restore the β_0 term in the NLO following the BLM precription [2]. Thus, in the NLO, we may switch off the gluino degrees of freedom. However, to get the $\{\beta\}$ expansion of the NNLO term in the form of Eq. (3.1c), we cannot use the quark degrees of freedom only. Indeed, in this case, we face a problem similar to that which arises in the process of $\{\beta\}$ decomposition of the pqQCD expression for d_2^{pqQCD} in Eq. (3.3) discussed above.

The $\{\beta\}$-expanded form for the d_3 term was obtained in Ref. [8] by means of a careful consideration of the analytical $\mathcal{O}(a_s^3)$ $\overline{\mathrm{MS}}$-scheme expression for the Adler function $D^{\mathrm{NS}}(a_s, \boldsymbol{n_f}, \boldsymbol{n_{\tilde g}})$ with the $\boldsymbol{n_{\tilde g}}$ QCD interacting MSSM gluino multiplets obtained in Refs. [25] and presented in Eqs. (A5b),(A5c)[3] together with the corresponding two-loop β function, $\beta(\boldsymbol{n_f}, \boldsymbol{n_{\tilde g}})$; see Eqs. (A1a) and (A1b).

Let us consider this procedure in more detail. The element $d_3[2]$, which is proportional to the maximum power β_0^2 in (3.1c), can be fixed in a straightforward way, using the results in Ref. [29]. Then, one should separate the contributions of $\beta_1\, d_3[0, 1]$ and of $\beta_0\, d_3[1]$ to the d_3 term. They both are linear in the number of quark flavors $\boldsymbol{n_f}$, and therefore, they could not be disentangled directly. Their separation is possible if one takes into account additional degrees of freedom, e.g., the gluino contributions mentioned above for both the quantities (the additional mark appears), namely, for the D^{NS} function from Eqs. (A5a)–(A5c) and for the first two coefficients of the β function from Eqs. (A1a) and (A1b). In this way, using two equations, one can get the explicit form for the functions $\boldsymbol{n_f} = n_f(\beta_0, \beta_1)$ and $\boldsymbol{n_{\tilde g}} = n_{\tilde g}(\beta_0, \beta_1)$. Finally, substituting these functions in $D = D(a_s, n_f(\beta_0, \beta_1), n_{\tilde g}(\beta_0, \beta_1))$, its $\{\beta\}$-expanded expression was obtained in Ref. [8],

$$\begin{aligned} D^{\mathrm{NS}}(a_s, n_f, n_{\tilde g}) = {} & 1 + a_s(3C_F) + a_s^2(3C_F)\cdot\left\{\frac{\mathrm{C_A}}{3} - \frac{\mathrm{C_F}}{2} + \left(\frac{11}{2} - 4\zeta_3\right)\beta_0(n_f, n_{\tilde g})\right\} \\ & + a_s^3(3C_F)\cdot\left\{\left(\frac{302}{9} - \frac{76}{3}\zeta_3\right)\beta_0^2(n_f, n_{\tilde g}) + \left(\frac{101}{12} - 8\zeta_3\right)\beta_1(n_f, n_{\tilde g})\right. \\ & + \left[\mathrm{C_A}\left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5\right) - \mathrm{C_F}(18 + 52\zeta_3 - 80\zeta_5)\right]\beta_0(n_f, n_{\tilde g}) \\ & \left. + \left(\frac{523}{36} - 72\zeta_3\right)\mathrm{C_A^2} + \frac{71}{3}\mathrm{C_A}C_\mathrm{F} - \frac{23}{2}\mathrm{C_F^2}\right\}, \end{aligned} \quad (3.7a)$$

[3]The NNLO analytical result for the gluino contribution evaluated in Ref. [25] was confirmed in Ref. [47].

with [see Eqs. (A1b)]

$$\beta_1(n_f, n_{\tilde{g}}) = \frac{34}{3}C_A^2 - \frac{20}{3}C_A\left(T_R n_f + \frac{n_{\tilde{g}}C_A}{2}\right) - 4\left(T_R n_f C_\text{F} + \frac{n_{\tilde{g}}C_A}{2}C_A\right). \quad (3.7b)$$

Note that, in order to write down the $\mathcal{O}(a_s^4)$ coefficient of D^{NS}, analytically evaluated in the $\overline{\text{MS}}$ scheme in Ref. [33] for the case of $SU(N_c)$ in a similar $\{\beta\}$-expanded form of Eq. (3.1d), it is necessary to perform additional calculations, which generalize this result to the case of $SU(N_c)$ with $n_{\tilde{g}}$ multiplets of gluinos. Then, one should combine this possible (but not yet existing) generalization with the already available analytical expression for the $\beta_2(n_f, n_{\tilde{g}})$ coefficient from Eq. (A1c) of the β function in this model, analytically obtained in the $\overline{\text{MS}}$ scheme in Ref. [48].

C. Does $\{\beta\}$ expansion have any ambiguities?

It is instructive to discuss here an attempt [5,7] to obtain the elements $d_n[\ldots]$ in a different way. This is based on the expression for D, rewritten in Ref. [49] for the usability of current five-loop computation in the form

$$D^{\text{EM}}(a_s) = 12\pi^2\left(\gamma_{\text{ph}}^{\text{EM}}(a_s) - \beta(a_s)\frac{d}{da_s}\Pi^{\text{EM}}(a_s)\right). \quad (3.8)$$

Here, $\Pi^{\text{EM}}(a_s) = \Pi^{\text{EM}}(L, a_s) \equiv d_R/(4\pi)^2 \sum_{i\geq 0}\Pi_i a_s^i$ is the polarization function of electromagnetic currents at $L \equiv \ln(Q^2/\mu^2) = 0$, and $\gamma_{\text{ph}}^{\text{EM}} \equiv 1/(4\pi)^2\sum_{j\geq 0}\gamma_j a_s^j$ is the anomalous dimension of the photon field. In our notation, Eq. (3.8) leads to the expansion for D^{NS},

$$D^{\text{NS}}(a_s) = 1 + 3C_\text{F}a_s + (12\gamma_2 + 3\beta_0\Pi_1)a_s^2 + (48\gamma_3 + 3\beta_1\Pi_1 + 24\beta_0\Pi_2)a_s^3 + \cdots, \quad (3.9)$$

where the ingredients of the expansion, γ_i, Π_j, were calculated in Ref. [49] up to $i = 4$, $j = 3$, and we take corresponding NS projection in the rhs of Eq. (3.8). The renormalization of the charge certainly contributes to the three-loop anomalous dimension γ_2. Therefore, it contains a β_0 term also (one can make sure from the inspection of the explicit formula for γ_2 in Eq. (3.12) in Ref. [49] and even in Eq. (10) in Ref. [20]). Taking into account the explicit form of γ_2 and Π_1 in (3.9), one can recalculate the well-known decomposition for D^{NS} in order $\mathcal{O}(a_s^2)$,

$$D^{\text{NS}}(a_s) = 1 + 3C_\text{F}\cdot a_s + 3C_\text{F}\cdot(\beta_0 d_2[1] + d_2[0])a_s^2 + O(a_s^3), \quad (3.10)$$

in full accordance with the result in Ref. [2] and Eq. (3.1b) (for the related discussions, see Ref. [17] as well).

Unfortunately the authors of Ref. [7] claim, basing on a formal correspondence, that the coefficient of β_0 is only the term Π_1/C_F in Eq. (3.9) (with the above notation at d_1 normalized by unity), while the "conformal term" is $4\gamma_2/C_\text{F}$ (see Eqs. (48a–48b) in Ref. [2]), which in reality is not true. The comparison of these terms

$$d_2[1] = \frac{11}{2} - 4\zeta_3 \approx 0.69177 \Leftrightarrow \Pi_1/C_\text{F} = \frac{55}{12} - 4\zeta_3 \approx -0.22489; \quad (3.11)$$

$$d_2[0] = d_2[0] = \frac{C_\text{A}}{3} - \frac{C_\text{F}}{2} \Leftrightarrow 4\gamma_2/C_\text{F} = \frac{11}{12}\beta_0 - \frac{C_\text{F}}{2} \quad (3.12)$$

shows that they differ even in sign in (3.11) (compare Π_1/C_F with $d_2[1]$). The considerations of Ref. [7] lead to a shift of the BLM scale Q^2_{BLM} in the opposite direction, $Q^2_{\text{BLM}} \geq Q^2$, in comparison with the standard value $Q^2_{\text{BLM}} = \exp(-d_2[1])Q^2 \approx Q^2/2$ [see the discussion after Eq. (5.3g) in Sec. V]. Moreover, we demonstrate in Eq. (3.12) that γ_2 is not conformal and depends on β_0.

IV. PARTIAL β-EXPANSION ELEMENTS FOR D, C, AND R

We extend here our knowledge about the β-expansion elements on the NS part of the Bjorken C^{Bjp} basing on CR Eq. (2.14b) for D^{NS} and $C^{\text{Bjp}}_{\text{NS}}$.

A. What constraints Crewther relation gives

In the case the β function has identically zero coefficients $\beta_i = 0$ for $i \geq 0$, the generalized CR (2.14b) returns to its initial form [27]

$$D_0^{\text{NS}}\cdot C_0^{\text{Bjp}} = \mathbb{1}, \quad (4.1)$$

where the expansions for the functions D_0^{NS} and C_0^{Bjp}, analogous to the ones of Eqs. (3.1b)–(3.1e), contain the coefficients of genuine content only, namely, $d_n(c_n) \equiv d_n[0](c_n[0])$. Equation (4.1) provides an evident relation between the genuine elements in any loops, namely,

$$c_n^{\text{NS}}[0] + d_n^{\text{NS}}[0] + \sum_{l=1}^{n-1} d_l^{\text{NS}}[0]c_{n-l}^{\text{NS}}[0] = 0, \quad (4.2)$$

where $d_n^{\text{NS}}[0] = d_1^{\text{NS}}\cdot d_n[0]$ and $c_n^{\text{NS}}[0] = c_1^{\text{NS}}\cdot c_n[0]$ in virtue of the normalization condition. From Eq. (4.2) at $n = 1$ immediately follows that $c_1^{\text{NS}} = -d_1^{\text{NS}}$. The relation (4.2) can be used to obtain the unknown genuine parts of the four-loop term $c_3^{\text{NS}}[0]$, through the four-loop results already known from the analysis in Ref. [8]:

$$c_3^{\rm NS}[0] = -d_3^{\rm NS}[0] + 2d_1^{\rm NS}d_2^{\rm NS}[0] - (d_1^{\rm NS})^3, \tag{4.3a}$$

or, in the other normalized terms,

$$c_3[0] = d_3[0] - 2d_1^{\rm NS}d_2[0] + (d_1^{\rm NS})^2. \tag{4.3b}$$

It is useful to relate the unknown elements $c_4^{\rm NS}[0]$, $d_4^{\rm NS}[0]$ in a five-loop calculation with the known elements of the four-loop results, viz.,

$$c_4^{\rm NS}[0] + d_4^{\rm NS}[0] = 2d_1^{\rm NS}d_3^{\rm NS}[0] - 3(d_1^{\rm NS})^2 d_2^{\rm NS}[0] + (d_2^{\rm NS}[0])^2 + (d_1^{\rm NS})^4. \tag{4.4}$$

Let us consider now the generalized CR in Eq. (2.14b), which includes the terms proportional to the conformal anomaly, $\beta(a_s)/a_s$, appearing due to violation of the conformal symmetry in the renormalized $SU(N_c)$ interaction (in the $\overline{\rm MS}$ scheme). As it was shown in Ref. [9], this relation can be rewritten in the multiple power representation

$$D^{\rm NS}\cdot C_{\rm NS}^{\rm Bjp} = \mathbb{1} + \frac{\beta(a_s)}{a_s}\cdot P(a_s) = \mathbb{1} + \frac{\beta(a_s)}{a_s}\cdot\sum_{n\geq1}\left(\frac{\beta(a_s)}{a_s}\right)^{n-1}\mathcal{P}_n(a_s), \tag{4.5}$$

where $\mathcal{P}_n(a_s)$ are the polynomials in a_s that can be expressed only in terms of the elements $d_k[\ldots]$, $c_k[\ldots]$. In this sense, $\mathcal{P}_n$ do not depend on the β function, all the charge renormalizations being accumulated by $(\beta(a_s)/a_s)^n$. We present the first two polynomials with factorized coefficients $-c_1^{\rm NS} = d_1^{\rm NS} = 3C_{\rm F}$:

$$\mathcal{P}_1(a_s) = -a_s d_1^{\rm NS}\{d_2[1] - c_2[1] + a_s[d_3[1] - c_3[1] - d_1^{\rm NS}(d_2[1] + c_2[1])] \tag{4.6a}$$

$$+ a_s^2[d_4[1] - c_4[1] - d_1^{\rm NS}(d_3[1] + c_3[1] + d_2[0]c_2[1] + d_2[1]c_2[0])]\}, \tag{4.6b}$$

$$\mathcal{P}_2(a_s) = a_s d_1^{\rm NS}\{d_3[2] - c_3[2] + a_s[d_4[1] - c_4[2] + d_1^{\rm NS}(c_3[2] + d_3[2])]\}, \tag{4.6c}$$

which were obtained and verified in N^{3}LO in Refs. [9,10] in another normalization. The construction of the β term on the rhs of (4.5) also creates constraints for combinations of the β-expansion elements. A few chains of these constraints were obtained in Ref. [9]. Further, we shall use the relation

$$d_2[1] - c_2[1] = d_3[0,1] - c_3[0,1] = \cdots = d_n[\underbrace{0,0,\ldots,1}_{n-1}] - c_n[\underbrace{0,0,\ldots,1}_{n-1}] = \left(\frac{7}{2} - 4\zeta_3\right), \tag{4.7}$$

which corresponds to Eq. (30) in Ref. [9].

If the terms $c_3[1]$, $d_3[1]$ and $c_4[2]$, $d_4[2]$ are missed in the $\{\beta\}$ expansion of $D^{\rm NS}$ and $C_{\rm NS}^{\rm Bjp}$, as in the variant of the expansion in Refs. [4–7], the structure of the generalized CR in Eqs. (4.6a)–(4.6c) is corrupted. That structure certainly contradicts the explicit results of analytical calculations of $D^{\rm NS}(a_s)$ and $C_{\rm NS}^{\rm Bjp}(a_s)$, preformed in the NNLO in Refs. [23–25] and in N^{3}LO in Ref. [33].

B. Nonsinglet parts of D and $C^{\rm Bjp}$

Following the approach discussed in Sec. III and taking into account a certain definition of the β-function coefficients in Eq. (2.3), we can obtain the β expansion for D–and C–functions. For the Adler function $D^{\rm NS}$, it reads

$$d_1^{\rm NS} = 3{\rm C_F};\quad d_1 = 1; \tag{4.8a}$$

$$d_2[1] = \frac{11}{2} - 4\zeta_3;\qquad d_2[0] = \frac{\rm C_A}{3} - \frac{\rm C_F}{2} = \frac{1}{3}; \tag{4.8b}$$

$$d_3[2] = \frac{302}{9} - \frac{76}{3}\zeta_3 \approx 3.10345;$$
$$d_3[0,1] = \frac{101}{12} - 8\zeta_3 \approx -1.19979; \tag{4.8c}$$

$$d_3[1] = {\rm C_A}\left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5\right) - {\rm C_F}(18 + 52\zeta_3 - 80\zeta_5) \approx 55.7005; \tag{4.8d}$$

$$d_3[0] = \left(\frac{523}{36} - 72\zeta_3\right){\rm C_A^2} + \frac{71}{3}{\rm C_A}C_{\rm F} - \frac{23}{2}{\rm C_F^2} \approx -573.9607, \tag{4.8e}$$

which differs from the ones presented in Ref. [9] (see its "natural form" in Appendix B), by the normalization factor only. It looks more convenient for a certain BLM task (the presentation corresponds to one in Ref. [8]) due to setting of the first PT coefficient, $d_1(c_1)$, equal to 1. Let us emphasize that gluinos are used here as a pure technical device to reconstruct the β-function expansion of the perturbative coefficients.

In this connection, we mention the relation $d_3[0,1] = d_n[0,\ldots,1] = d_2[1]$ proposed in Ref. [5] and based on a "special degeneracy of the coefficients" suggested there (see Eq. (6) in Ref. [5]) in an analogy with the perturbative series rearrangement, $d_i \to d'_i$ under the change of the coupling renormalization scale, $a(\mu^2) \to a'(\mu'^2)$ [see the discussions in Sec. V A below]. This rearrangement has an *outside* reason with respect to d_i and "does not know" about the *intrinsic* structure of the initial coefficient d_i under consideration. This relation is artificial, and for this reason, it is not supported by the direct calculations. The explicit result of this rearrangement is presented in Eq. (5.3a) and below; it is the initial step for any BLM optimization procedure that will be discussed in Sec. V in detail.

Let us compare now Eqs. (4.8c)–(4.8e) with the results presented in Ref. [7] and based on the interpretation of the term $(\underline{48\gamma_3} + 3\beta_1\Pi_1 + \underline{24\beta_0\Pi_2})a_s^3$ in the presentation of (3.9). The first and the third terms of the sum form the term proportional to β_0^2,

$$\underline{48\gamma_3} + \underline{24\beta_0\Pi_2} \longrightarrow \beta_0^2\left(\frac{302}{9} - \frac{76}{3}\zeta_3 = d_3[2]\right), \qquad (4.9)$$

that can be unambiguously obtained by extracting the n_f^2 terms in γ_3 and the β_0 term in Π_2; see the corresponding explicit expressions in Refs. [49]. The second term there, $\beta_1\Pi_1$, certainly contributes to the value of the element $d_3[0,1]$. There are other terms, proportional to β_1, in both the γ_3 and $\beta_0\Pi_2$ terms that also contribute to $d_3[0,1]$. However, these required terms cannot be separated unambiguously from those terms that are proportional to β_0. The final explicit expressions given in Ref. [49] are not sufficient for this separation, as it was already discussed in Sec. III B.

Let us consider the β expansion of the Bjorken coefficient function $C_{\mathrm{NS}}^{\mathrm{Bjp}}$ of the DIS sum rules. Based on CR (4.2) for $n = 2$ and $n = 3$ and the already fixed $d_2[0]$ and $d_3[0]$-terms, we get expression (4.3b) for the $c_2[0]$ and $c_3[0]$ elements of $C_{\mathrm{NS}}^{\mathrm{Bjp}}$, namely, $c_3[0] = d_3[0] - 2d_1^{\mathrm{NS}} d_2[0] + (d_1^{\mathrm{NS}})^2$; see the explicit expression in (4.10e). The knowledge of $c_3[0]$ allow us to fix all other elements $c_3[\ldots]$ of the PT coefficient c_3 without involving additional degrees of freedom [9]. It is instructive to consider this in detail. Indeed, the terms $c_3[0]$ as well as the coefficient $c_3[2]$ of the β_0^2 (maximum power of n_f) can be found independently. Therefore, the Casimir structure of the rest of c_3, $c_3 - c_3[0] - \beta_0^2 c_3[2]$, contains five basis elements (we factor out $c_1^{\mathrm{NS}} = -3C_{\mathrm{F}}$):

$$c_3 - c_3[0] - \beta_0^2 c_3[2] : \begin{cases} C_{\mathrm{F}}^2, C_{\mathrm{A}}^2, C_{\mathrm{A}}C_{\mathrm{F}}, T_{\mathrm{R}}n_f C_{\mathrm{F}}, T_{\mathrm{R}}n_f C_{\mathrm{A}} \\ \beta_1, \beta_0 \end{cases}$$

This Casimir structure of the rest should be equated to the β expansion of the one [see decomposition (3.1c)], $c_3[0,1]\cdot\beta_1 + (x\cdot C_{\mathrm{F}} + y\cdot C_{\mathrm{A}})\cdot\beta_0$. It contains three unknown coefficients $c_3[0,1], x, y$.

The C_{F}^2 terms in the explicit result for c_3 [38] [see Eq. (A7c)] and in the expression for $c_3[0]$ in Eq. (4.10e) coincide with one another; therefore, the term $\frac{1}{2}C_{\mathrm{F}}^2$ is canceled in the rest. This confirms the fact that its β expansion does not contain C_{F}^2. So, we have four constraints (not five) for the three coefficients $c_3[0,1], x, y$. This overdetermined system is nevertheless a system of simultaneous equations; the fact provides us with an *independent confirmation* of this β expansion. The explicit form of the elements was first obtained in Ref. [9]; below, we present them at the same normalization as Eqs. (4.8c)–(4.8e) [cf. (4.8e) with (4.10e)]:

$$c_1^{\mathrm{NS}} = -3C_{\mathrm{F}}; \qquad c_1 = 1; \qquad (4.10a)$$

$$c_2[1] = 2; \qquad c_2[0] = \left(\frac{1}{3}C_A - \frac{7}{2}C_{\mathrm{F}}\right) = -\frac{11}{3} = -3.6(6); \qquad (4.10b)$$

$$c_3[2] = \frac{115}{18} = 6.38(8);$$
$$c_3[0,1] = \left(\frac{59}{12} - 4\zeta_3\right) \approx 0.10844; \qquad (4.10c)$$

$$c_3[1] = -\left(\frac{166}{9} - \frac{16}{3}\zeta_3\right)C_{\mathrm{F}} - \left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5\right)C_A \approx 39.9591; \qquad (4.10d)$$

$$c_3[0] = \left(\frac{523}{36} - 72\zeta_3\right)C_A^2 + \frac{65}{3}C_{\mathrm{F}}C_A + \frac{C_{\mathrm{F}}^2}{2} \approx -560.627. \qquad (4.10e)$$

The same results can be obtained if one fixes first the element $c_3[0,1] = d_3[0,1] - d_2[1] + c_2[1]$ from relation (4.7); the latter originates from another source—the symmetry-breaking term proportional to $\beta(a_s)$ in the generalized CR. Therefore, the results (4.10b)–(4.10c) are in mutual agreement with both the terms on the rhs of CR and can be obtained independently from each of them.

These elements of decomposition in (4.10) allow one to make a *new prediction* for the light gluino contribution to $C_{\mathrm{NS}}^{\mathrm{Bjp}}$. Indeed, the effects of charge renormalization are manifesting themselves through the elements of $c[\ldots]$—the coefficients of the β-function products [named B^i in the matrix representation discussed in Sec. III A after Eq. (3.2c)]. They are formed following gauge interactions. The effect of various degrees of freedom, namely a gluino, which reveals itself only in intrinsic loops, changes the content of the β coefficients β_i with the corresponding mark, namely, $\boldsymbol{n_{\tilde{g}}}$. Therefore, to obtain $C^{\mathrm{Bjp}} \to C^{\mathrm{Bjp}}(a_s, n_f, n_{\tilde{g}})$ with the light MSSM gluino, one should replace the β coefficients $\beta_i \to \beta_i(n_f, n_{\tilde{g}})$ and compose them with the elements from Eq. (4.10a)–(4.10e),

TABLE I. The Table exemplifies the structure of a few first coefficients r_m of the conventional expansion of the R ratio. Every coefficient r_m contains a number of $d_k (k \leq m)$ terms in its expansion, which are shown in the corresponding row. Here $r_m = T^{mk} d_k$ (summation in $k = 1, \ldots, m$ is assumed), where T^{mk} are the table entries. The proportional to the powers of $(\pi\beta_0)^2$ analytical continuation effects are marked by gray, other ones are marked by bold font.

	d_1	d_2	d_3	d_4	d_5	d_6
r_1	$\mathbf{1}$					
r_2	0	$\mathbf{1}$				
r_3	$-\frac{(\pi\beta_0)^2}{3}$	0	$\mathbf{1}$			
r_4	$0 - \frac{5\pi^2}{6}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3} 3$	0	$\mathbf{1}$		
r_5[a]	$\frac{(\pi\beta_0)^4}{5} - \frac{\pi^2}{2}\beta_1^2 - \pi^2\beta_0\beta_2$	$0 - \frac{7\pi^2}{3}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3} 6$	0	$\mathbf{1}$	
r_6	$0 - \frac{77\pi^4}{60}\beta_0^3\beta_1 - \frac{7\pi^2}{6}\beta_1\beta_2 - \frac{4\pi^2}{3}\beta_0\beta_3$	$-\frac{(\pi\beta_0)^4}{5} 5 - \frac{4\pi^2}{3}\beta_1^2 - \frac{8\pi^2}{3}\beta_0\beta_2$	$0 - \frac{9\pi^2}{2}\beta_0\beta_1$	$-\frac{(\pi\beta_0)^2}{3} 10$	0	$\mathbf{1}$

[a]This expression for r_5 was presented first in Ref. [51].

$$C_{\mathrm{NS}}^{\mathrm{Bjp}}(a_s, n_f, n_{\tilde{g}}) = 1 + a_s(-3C_F) \tag{4.11a}$$

$$+ a_s^2(-3C_F) \cdot \left\{ \frac{1}{3} \mathrm{C}_A - \frac{7}{2} \mathrm{C}_\mathrm{F} + 2\beta_0(n_f, n_{\tilde{g}}) \right\} \tag{4.11b}$$

$$+ a_s^3(-3C_F) \cdot \left\{ \frac{115}{18} \beta_0^2(n_f, n_{\tilde{g}}) + \left(\frac{59}{12} - 4\zeta_3 \right) \beta_1(n_f, n_{\tilde{g}}) - \left[\left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5 \right) \mathrm{C}_A + \left(\frac{166}{9} - \frac{16}{3}\zeta_3 \right) \mathrm{C}_\mathrm{F} \right] \beta_0(n_f, n_{\tilde{g}}) + \left(\frac{523}{36} - 72\zeta_3 \right) \mathrm{C}_A^2 + \frac{65}{3} \mathrm{C}_\mathrm{F} C_A + \frac{\mathrm{C}_\mathrm{F}^2}{2} \right\}. \tag{4.11c}$$

This logic can be reverted: the values of $c_3[0], c_3[0,1]$ and then the CR can be checked from the direct calculation of $C_{\mathrm{NS}}^{\mathrm{Bjp}}(a_s, n_f, n_{\tilde{g}})$ with the MSSM massless gluino.

C. Singlet parts and the R ratio

Here, we present the singlet part of the Adler function, d_4, that can be obtained based on the result for c_4 of $C_{\mathrm{S}}^{\mathrm{Bjp}}$ and CR [34],

$$d_4^S = \beta_0(n_f) \cdot d_4^S[1] + d_4^S[0], \tag{4.12}$$

$$d_4^S[0] = \left(-\frac{13}{64}\zeta_3 - \frac{5}{32}\zeta_5 + \frac{205}{1536} \right) C_A + \left(-\frac{1}{4}\zeta_3 + \frac{5}{8}\zeta_5 - \frac{13}{64} \right) C_F, \tag{4.13}$$

$$d_4^S[1] = -\frac{13}{32}\zeta_3 - \frac{1}{8}\zeta_3^2 + \frac{5}{16}\zeta_5 + \frac{149}{576}, \tag{4.14}$$

$$c_4^S = c_4^S[0] + \beta_0(n_f) \cdot c_4^S[1], \tag{4.15}$$

$$c_4^S[0] = \left(\frac{13}{64}\zeta_3 + \frac{5}{32}\zeta_5 - \frac{205}{1536} \right) C_A + \left(\frac{1}{16}\zeta_3 - \frac{5}{8}\zeta_5 + \frac{37}{128} \right) C_F, \tag{4.16}$$

$$c_4^S[1] = -\frac{119}{1152} + \frac{67}{288}\zeta(3) + \frac{1}{8}\zeta(3)^2 - \frac{35}{144}\zeta(5). \tag{4.17}$$

The integral transform $D \to R_{e^+e^-}$,

$$R_{e^+e^-}(s) \equiv R(s, \mu^2 = s) = \frac{1}{2\pi i} \int_{-s-i\varepsilon}^{-s+i\varepsilon} \frac{D^{\mathrm{EM}}(\sigma/\mu^2; a_s(\mu^2))}{\sigma} d\sigma \Big|_{\mu^2 = s} = \left(\sum_i q_i^2 \right) d_R \left(1 + \sum_{m \geq 1} r_m^{\mathrm{NS}} a_s^m(s) \right) + \left(\sum_i q_i \right)^2 \frac{d^{abc} d^{abc}}{d_R} \sum_{n \geq 3} r_n^{\mathrm{S}} a_s^n(s), \tag{4.18}$$

can be realized as a linear relation by means of the matrix T, $r_j = T^{ji} d_i$, or for the vector representation $R = TD = \sum a_s^j T^{ji} d_i$. The triangular matrix T of the relation can be obtained at any fixed order of perturbative theory [50]. The elements of this matrix below the units on the diagonal contain so-called kinematic "π^2 terms" multiplied by the β-function coefficients[4]; see an example of T^{ji} in Table I. Taking into account that the β structure of the normalized coefficients $r_i = r_i^{\mathrm{NS}}/r_1^{\mathrm{NS}}$ is like that for the coefficients d_i, Eqs. (3.1a)–(3.1d), one can rewrite the results from the matrix in Table I,

[4]These terms can be obtained for any order of perturbative theory (constrained mainly by the value of RAM) with a Mathematica routine constructed by V. L. Khandramai and S. V. Mikhailov.

$$r_0 = d_0; \quad r_1^{\rm NS} = d_1^{\rm NS}; \quad r_1 = 1; \quad r_2 = d_2; \tag{4.19a}$$

$$r_3[2] = d_3[2] - \frac{\pi^2}{3}; \qquad r_3^{\rm S}[2] = d_3^{\rm S}[2]; \tag{4.19b}$$

$$\begin{aligned} r_4[3] &= d_4[3] - \pi^2 d_2[1]; \\ r_4[2] &= d_4[2] - \pi^2 d_2[0]; \\ r_4[1,1] &= d_4[1,1] - \frac{5}{6}\pi^2; \end{aligned} \tag{4.19c}$$

$$\begin{aligned} &r_5[4] = d_5[4] + \frac{\pi^4}{5} - 2\pi^2 d_3[2]; \\ &r_5[0,2] = d_5[0,2] - \frac{\pi^2}{2}; \\ &r_5[2,1] = d_5[2,1] - \pi^2\left(\frac{7}{3}d_2[1] + d_3[0,1]\right); \\ &r_5[1,0,1] = d_5[1,0,1] - \pi^2; \quad r_5[1,1] = d_5[1,1] - \frac{7}{3}\pi^2 d_2[0]; \\ &r_5[3] = d_5[3] - 2\pi^2 d_3[1]; \quad r_5[2] = d_5[2] - 2\pi^2 d_3[0], \end{aligned} \tag{4.19d}$$

while the other elements in r_i coincide with ones in d_i ($i \le 5$). A similar matrix T^S_{nl} that relates the coefficients $r_n^{\rm S}$ and $d_l^{\rm S}$ can be constructed as well. However, in this work, we will not consider the π^2-dependent effects of analytical continuation, which in the singlet case appear first at the $\mathcal{O}(a_s^5)$ level. Further, we shall use Eqs. (4.19a)–(4.19c) to construct PT-optimized series for R.

V. BLM AND PMC PROCEDURES AND THE RESULTS

A. General basis

The reexpansion of the running coupling $\bar{a}(t) = a(\Delta, a')$ and its powers in terms of $t - t' = \Delta = \ln(\mu^2/\mu'^2)$ and new coupling a' reads

$$\begin{aligned} \bar{a}(t) = a(\Delta, a') &= a' - \beta(a')\frac{\Delta}{1!} + \beta(a')\partial_{a'}\beta(a')\frac{\Delta^2}{2!} \\ &\quad + \beta(a')\partial_{a'}(\beta(a')\partial_{a'}\beta(a'))\frac{\Delta^3}{3!} + \cdots \\ &= \exp(-\Delta\beta(\bar{a})\partial_{\bar{a}})\bar{a}|_{\bar{a}=a'}, \end{aligned} \tag{5.1}$$

which is the way to write the corresponding RG solution for $a(t)$ through the operator $\exp(-\Delta\beta(a)\partial_a)[\ldots]|_{a=a'}$) (see Ref. [8] and refs therein). The shift of the logarithmic scale Δ in its turn can be expanded in perturbative series in powers of $a'\beta_0$,

$$\begin{aligned} &t' \equiv t - \Delta, \\ &\Delta \equiv \Delta(a') = \mathbf{\Delta_0} + a'\beta_0\mathbf{\Delta_1} + (a'\beta_0)^2\mathbf{\Delta_2} + \cdots, \end{aligned} \tag{5.2}$$

where the argument of the new coupling a' depends on $t' = t - \Delta$. It is sufficient to take this renormalization scale for the a' argument, which corresponds to the solution on the previous step, rather than to solve the exact equation $a(t - \Delta(a')) = a'$. Reexpansion a in terms of a' leads to rearrangement of the series of perturbative expansion for the RGI quantity $D^a(C^{\rm Bjp})$, $a^i d_i \to a'^i d'_i$, where the rhs are expressed in a rather long but evident formula. In the square brackets below, we write them explicitly:

$$\begin{aligned} &a^1 \cdot d_1 \to a'^1 \cdot [d'_1 = 1]; \\ &a^2 \cdot d_2 \to a'^2 \cdot [d'_2 = \beta_0 d_2[1] + d_2[0] - \beta_0\mathbf{\Delta_0}]; \end{aligned} \tag{5.3a}$$

$$\begin{aligned} a^3 \cdot d_3 \to a'^3 \cdot [d'_3 = \beta_0^2(d_3[2] - 2d_2[1]\mathbf{\Delta_0} + \mathbf{\Delta_0^2}) \\ + \beta_1(d_3[0,1] - \mathbf{\Delta_0}) + \end{aligned} \tag{5.3b}$$

$$\beta_0(d_3[1] - 2d_2[0]\mathbf{\Delta_0}) + d_3[0] - \beta_0^2\mathbf{\Delta_1}]; \tag{5.3c}$$

$$\begin{aligned} a^4 \cdot d_4 \to a'^4 \cdot \Big[d'_4 = \beta_0^3(d_4[3] - 3d_3[2]\mathbf{\Delta_0} + 3d_2[1]\mathbf{\Delta_0^2} - \mathbf{\Delta_0^3} - 2(\mathbf{\Delta_0} - d_2[1])\mathbf{\Delta_1}) \\ + \beta_1\beta_0\left(d_4[1,1] - (3d_3[0,1] + 2d_2[1])\mathbf{\Delta_0} + \frac{5}{2}\mathbf{\Delta_0^2} - \mathbf{\Delta_1}\right) + \beta_2(d_4[0,0,1] - \mathbf{\Delta_0}) + \end{aligned} \tag{5.3d}$$

$$\begin{aligned} &\beta_0^2(d_4[2] - 3d_3[1]\mathbf{\Delta_0} + 3d_2[0]\mathbf{\Delta_0^2} - 2d_2[0]\mathbf{\Delta_1}) \\ &\quad + \beta_1(d_4[0,1] - 2d_2[0]\mathbf{\Delta_0}) + \end{aligned} \tag{5.3e}$$

$$\beta_0(d_4[1] - 3d_3[0]\mathbf{\Delta_0}) + d_4[0] - \beta_0^3\mathbf{\Delta_2}\Big]; \tag{5.3f}$$

……

$$a^n \cdot d_n \to a'^n \cdot [d'_n = \beta_0^{n-1} d_n[n-1] + \ldots]. \tag{5.3g}$$

The standard BLM fixes the scale $\mathbf{\Delta_0}$ by the requirement $\mathbf{\Delta_0} = d_2[1]$, accumulating one-loop renormalization of charge just in this new scale [2], at the same time the coefficient $d_2 \to d_2[0]$—its "conformal part." Numerically,

$$\mathbf{\Delta_0} = d_2[1] = \frac{11}{2} - 4\zeta_3 = 0.69177\ldots \approx \ln(2) = 0.69314\ldots; \tag{5.4}$$

therefore, $Q^2_{\rm BLM} = \exp(-\mathbf{\Delta_0})Q^2 \approx Q^2/2$.

High-order generalization of BLM can be realized in different ways requiring consequently certain equations for the partial shifts $\{\mathbf{\Delta}_i\}$. The system of Eqs. (5.3a)–(5.3g) for d'_i is the basis to construct different BLM generalizations. It is instructive to consider these coefficients $\{d'_i\}$ after the first BLM step; taking $\mathbf{\Delta_0} = d_2[1]$, one obtains

$$d'_2 = d_2[0]; \tag{5.5a}$$

$$d'_3 = \beta_0^2\underline{(d_3[2] - d_2[1]^2)} + \beta_1\underline{\underline{(d_3[0,1] - d_2[1])}} + \beta_0(d_3[1] - 2d_2[0]d_2[1]) + d_3[0] - \beta_0^2\Delta_1; \tag{5.5b}$$

$$d'_4 = \beta_0^3\underline{(d_4[3] - 3d_3[2]d_2[1] + 2d_2[1]^3)} + \beta_2\underline{\underline{(d_4[0,0,1] - d_2[1])}} \times \beta_1\beta_0(d_4[1,1] - 3d_3[0,1]d_2[1] + d_2[1]^2/2 - \mathbf{\Delta_1}) + \tag{5.5c}$$

$$\beta_0^2(d_4[2] - 3d_3[1]d_2[1] + 3d_2[0]d_2[1]^2 - 2d_2[0]\mathbf{\Delta_1}) + \tag{5.5d}$$

$$\beta_1(d_4[0,1] - 2d_2[0]d_2[1]) + \tag{5.5e}$$

$$\beta_0(d_4[1] - 3d_3[0]d_2[1]) + d_4[0] - \beta_0^3\Delta_2; \tag{5.5f}$$

$$\dots\dots$$

$$d'_n = \beta_0^{n-1}d_n[n-1] + \dots \tag{5.5g}$$

The detailed analysis of the d'_i structure was made in Ref. [8] in Sec. 5. Here, we mention a common property of this transform—to obtain the rearrangement of the coefficient at an order $n+1$, $d_{n+1} \to d'_{n+1}$, one should know its β structure up to the previous order n. For the partial case of relation $d_{n+1}[n] = (d_2[1])^n$, the β_0^n terms are canceled (underlined terms) in all the orders even due to the first BLM step. Correspondingly, the special conditions $d_i[0,\dots,1] = d_2[1]$ will remove the next terms with the leading coefficient β_{i-2} in every order; see the double underlined terms in Eqs. (5.5b) and (5.5c). The latter conditions were proposed in Ref. [5] [see the discussion in Sec. IV B here after Eq. (4.8e)], though both of the above hypotheses are far from the results of the direct calculations at $\mathcal{O}(a_s^3)$ in (4.8); really

$$d_3[2] - d_2[1]^2 \approx 3.1035 - 0.4785;$$
$$d_3[0,1] - d_2[1] \approx 1.1998 - 0.6918. \tag{5.6}$$

Even more, in QCD, the elements $d_{n+1}[n]$ grow as $n!$ due to renormalon contributions [29], and the role of these terms becomes more and more important. To construct the next steps of the PT optimization with $\mathbf{\Delta_1}, \mathbf{\Delta_2}, \dots$, one should get more detailed knowledge or provide a hypothesis about the different contributions in d'_n.

B. seBLM and PMC procedures

One of the hypotheses mentioned above is based on the empirical relation between the QCD β-function coefficients β_i, $\beta_i \sim \beta_0^{i+1}$. This can be easily verified for perturbative quenched QCD ($n_f = 0$) numerically, and this works in the range of $n_f = 0 \div 5$ of quark flavors for the all known β coefficients; compare the expressions in Eqs. (A1a)–(A1c),

$$\beta_i \sim \beta_0^{i+1}, \qquad c_i = \beta_i/\beta_0^{i+1} = \mathcal{O}(1). \tag{5.7}$$

This relation allows one to set a hierarchy of contributions in order of the "large value of β_0" [$\beta_0 = 11(9)$ at $n_f = 0(3)$] [8]. Of course, relation (5.7) should be broken at some large enough order of expansion i_0 in virtue of expected Lipatov-like asymptotics for the β function $\beta_i \sim (i!)\beta_0^{i+1}$. Therefore, this hierarchy has a restricted field of application that describes the term "practical approach" in the title of Ref. [8].

For this hierarchy, the most important terms are in the powers of β_0 contributions leading of an order $(\beta_0 a_s)^n/\beta_0$, which are underlined below in Eqs. (5.8a)–(5.8h). For illustration, we shall use the $R^{\rm NS}(s)$ ratio, taking into account the result (5.5) for D and relations in Eq. (4.19b)–(4.19d):

$$r'_2 = d_2[0], \tag{5.8a}$$

$$r'_3 = \beta_0^2\underline{(d_3[2] - d_2[1]^2 - \pi^2/3)} + \beta_1\underline{(d_3[0,1] - d_2[1])} \tag{5.8b}$$

$$+ \underline{\underline{\beta_0(d_3[1] - 2d_2[0]d_2[1])}} - \beta_0^2\Delta_1 + d_3[0]; \tag{5.8c}$$

$$r'_4 = \beta_0^3\underline{(d_4[3] - 3d_3[2]d_2[1] + 2d_2[1]^3 - \pi^2 d_2[1])} + \beta_2\underline{(d_4[0,0,1] - d_2[1])} \times \beta_1\beta_0\underline{\underline{(d_4[1,1] - 3d_3[0,1]d_2[1] + d_2[1]^2/2 - 5/6\pi^2 - \mathbf{\Delta_1})}} + \tag{5.8d}$$

$$\beta_0^2\underline{\underline{(d_4[2] - 3d_3[1]d_2[1] + 3d_2[0]d_2[1]^2 - \pi^2 d_2[0] - 2d_2[0]\mathbf{\Delta_1})}} + \tag{5.8e}$$

$$\beta_1\underline{\underline{(d_4[0,1] - 2d_2[0]d_2[1])}} + \tag{5.8f}$$

$$\beta_0\underline{\underline{(d_4[1] - 3d_3[0]d_2[1])}} - \beta_0^3\Delta_2 + d_4[0]; \tag{5.8g}$$

$$r'_n = \underline{\beta_0^{n-1}d_n[n-1] + \dots} + \dots \tag{5.8h}$$

The less important terms are suppressed by β_0^{-1} in every order. These are the terms $(\beta_0 a_s)^n/\beta_0^2$. They are double underlined in (5.8c), (5.8e), (5.8f), and so on. Following the hierarchy, one fixes the values of $\Delta_1, \boldsymbol{\Delta}_2, \ldots$, consequently nullifying at first the most important (single-underlined) β terms in every order. After that, the procedure repeats with the less important terms (double underlined) in all orders, etc. This procedure was called seBLM, and its result was presented in detail in Sec. 6 of Ref. [8] [see Eqs. (6.7) and (6.8) there]. The discussed hierarchy can also be used for generalization of the NNA approximation; see Appendix C in Ref. [50].

The above invented hierarchy ignores a possible difference of values of the elements $d_n[\ldots]$, tacitly suggesting that they are of the same order of magnitude. Of course, one can abandon the suggestion of the hierarchy and can remove *all the* β *terms in one mold* consequently order by order. This approach leads to other values of $\Delta_i = \bar{\boldsymbol{\Delta}}_i$,

$$\bar{\boldsymbol{\Delta}}_0 = d_2[1]; \tag{5.9a}$$

$$\bar{\boldsymbol{\Delta}}_1 = \frac{1}{\beta_0^2}[\beta_0^2(d_3[2] - d_2^2[1] - \pi^2/3) + \beta_1(d_3[0,1] - d_2[1]) + \beta_0\underline{\underline{(d_3[1] - 2d_2[1]d_2[0])}}] \tag{5.9b}$$

$$\bar{\boldsymbol{\Delta}}_2 = \frac{1}{\beta_0^3}\Big[\beta_0^3(d_4[3] - 3d_2[1]d_3[2] + 2(d_2[1])^3 - \pi^2 d_2[1]) + \beta_2(d_4[0,0,1] - d_2[1]) + \beta_0\beta_1\left(d_4[1,1] - 3d_3[0,1]d_2[1] + \frac{3}{2}(d_2[1])^2 - d_3[2] - \pi^2/2\right) + \beta_1^2/\beta_0(d_2[1] - d_3[0,1]) + \beta_1(\underline{\underline{\ldots}}) + \ldots\Big], \tag{5.9c}$$

which differ by the underlined "suppressed in the $1/\beta_0$" terms from the previous ones in Ref. [8]. The complete form for Δ_2 looks cumbersome, and it is outlined in Appendix C. The procedure like this was called PMC later on [3], though for both the cases, seBLM and corrected PMC, the final PT series has the same conformal terms $d_n[0]$ as the coefficients of new expansion. The new normalization scale s' follows from Eq. (5.2), taking into account certain expressions for Δ_i in Eqs. (5.9a)–(5.9c),

$$R_{e^+e^-}(s) = \left(\sum_i q_i^2\right)\cdot d_A R^{\rm NS} + \left(\sum_i q_i\right)^2 \cdot d_A R^{\rm S}$$
$$R^{\rm NS}(s) = 1 + 3C_F\{a(s') + d_2[0]\cdot a^2(s') + d_3[0]\cdot a^3(s') + d_4[0]\cdot a^4(s') + \ldots\} \tag{5.10a}$$

$$\ln(s/s') = \bar{\Delta}_0 + a'\beta_0\bar{\Delta}_1 + (a'\beta_0)^2\bar{\Delta}_2 + \ldots. \tag{5.10b}$$

The formulae of Eqs. (5.9a)–(5.9c) and Eqs. (5.10a), (5.10b) are the main results of these subsections.

C. Numerical estimates, discussion of PMC/seBLM results

Here we apply the results of the described above procedure for the numerical estimates of the expansion coefficients for a few processes starting with the nonsinglet part $R^{\rm NS}$ of the $R_{e^+e^-}(s)$ ratio. The corresponding singlet part $R^{\rm S}$ can be optimized independently; moreover, it is not very important numerically. For the sake of illustration, we put the value $n_f = 3$ for all estimates below. At the very beginning, we have the following numerical structure of r_i:

$$r_2 = \beta_0\cdot 0.69 + \frac{1}{3} \approx 6.56; \tag{5.11a}$$

$$r_3 = -\beta_0^2\cdot 0.186 - \beta_1\cdot 1.2 + \beta_0\cdot 55.70 - 573.96 \approx -164.5 \tag{5.11b}$$

$$-15.1 - 76.8 + 501.3 - 573.96; \qquad r_4 \approx -6840.29. \tag{5.11c}$$

At the first BLM setting $\bar{\Delta}_0 \approx 0.69$, $a_s(s) \to a'_s = a_s(se^{-0.692} \approx s/2)$, we obtain for the coefficients r'_2, r'_3—Eqs. (5.12a) and (5.12b)—the explicit result of the BLM procedure. The value of the second coefficient r'_2 diminishes by an order of magnitude, while r'_3 becomes moderately larger, compare (5.11b) with (5.12b),(5.13a),

$$r'_2 = \frac{1}{3}; \tag{5.12a}$$

$$r'_3 = -\beta_0^2\cdot 0.665 - \beta_1\cdot 1.892 + \beta_0\cdot 55.24 - 573.96 \approx -\underline{251.7}; \tag{5.12b}$$

$$-53.86 - 121.0 + 497.1 - 573.96 \qquad r'_4 \approx -8559.89. \tag{5.12c}$$

At the second step (PMC), we obtain $\bar{\Delta}_1 \approx 3.98$ following Eqs. (5.9b) and (5.2),

$$r''_3 \approx -\underline{573.96}, \qquad \bar{\Delta}_1 \approx 3.98, \tag{5.13a}$$

$$r''_4 \approx -11066.1, \tag{5.13b}$$

$$a'_s \to a''_s = a_s(s \cdot e^{-0.692-3.98\beta_0 a'_s(s)}), \tag{5.13c}$$

while $r''_3 = d_3[0]$ following the main aim of PMC; see Eq. (5.10a). Because of the strong suppression of the normalization scale by a factor of $\exp[-0.692 - 3.98\beta_0 a'_s(s)]$, the applicability of PT is shifted to the region of very large s; simultaneously, the coefficient r''_3 increases three times [cf. (5.11b)]. So this procedure makes the convergence of PT worse.

Within the same framework, we obtain for the coefficient of the Bjorken function $C^{\mathrm{Bjp}}_{\mathrm{NS}}$:

$$c_2 = \beta_0 \cdot 2 - \frac{11}{3} = 14.3(3); \tag{5.14a}$$

$$c_3 = \beta_0^2 \cdot 6.39 + \beta_1 \cdot 0.1084 + \beta_0 \cdot 39.95 - 560.63 \\ \approx 323.44; \tag{5.14b}$$

$$517.5 + 6.9401 + 359.63 - 560.63; \\ c_4 \approx 11247.97. \tag{5.14c}$$

At the first BLM step, we do not obtain a significant profit in the first coefficient $c_2 \to c'_2$, as it was in the previous case of r'_2. But the next-order coefficient $c_3 \approx 352.05$ in (5.14b) diminished by two orders of magnitude, $c_3 \to c'_3 \approx 3.444$ at $a_s(Q^2) \to a'_s = a_s(Q^2 e^{-2} \approx Q^2 \cdot 0.135)$,

$$c'_2 = -\frac{11}{3}; \tag{5.15a}$$

$$c'_3 = \beta_0^2 \cdot 2.389 - \beta_1 \cdot 1.892 + \beta_0 \cdot 54.63 - 560.63 \approx \underline{3.444}; \tag{5.15b}$$

$$193.5 - 121.06 + 491.63 - 560.63, \\ c'_4 \approx 6361.0. \tag{5.15c}$$

It is interesting that the far fourth coefficient c_4 (5.14c) reduces twice, $c_4 \to c'_4$ (5.15c). At the second step (PMC), $\bar{\Delta}_1 \approx 7.32$, and $a'_s \to a''_s = a_s(Q^2 \cdot \exp[-2 - 7.32\beta_0 a'(Q^2)])$; so the region of applicability of PT is shifted far from the scale of a few GeV^2. While the value of $|c''_3|$ goes up to the previous order of magnitude, compare (5.15b) to (5.16),

$$c''_2 = -\frac{11}{3}; \qquad c''_3 \approx -\underline{560.63}. \tag{5.16}$$

It is instructive to compare this result with one from seBLM (Sec. V B), where we remove the first two terms in (5.15b), converting them into the normalization scale and holding the last two terms in c''_3. For this prescription, we obtain $\Delta_1 \approx 1.25$,

$$a'_s \to a''_s = a_s(Q^2 \exp[-2 - 1.25\beta_0 a'(Q^2)]) \quad \text{and} \\ c''_3 \approx -69,$$

that looks moderate but is not optimal yet in the sense of series convergence.

Both aforementioned examples demonstrate better convergence at the first BLM step but fail for the optimization of PT at the second PMC step. The reason is the different sign of the terms of $r_n(c_n)$; see the discussion in Secs. 6 and 7 in Ref. [8]. It is clear that one should not remove and absorb *all the β terms* for the PT optimization but leave a part of them for complete cancellation with the $d_n[0]$ term. We shall treat the circumstances in this way in the next section.

VI. OPTIMIZATION OF THE GENERALIZED BLM PROCEDURE

Indeed, it is not mandatory to absorb all the β terms as a whole into the new scale $\Delta_1(\Delta_i)$ following BLM/PMC but to take instead only those parts of it that are appropriate for optimization (nullification) of the current-order coefficient $r_3(r_{i+2})$. At the same time, one should care for the size of the Δ_i–PT coefficients for the shift of scale Δ in (5.2)—not to violate just this expansion.

Let us consider the optimization of R^{NS} at the second BLM step, starting with the first step expressions in Eqs. (5.12a)–(5.12c) and using the general results in (5.8c), (5.8e), and (5.8d). This expression for r''_3 can be rewritten as

$$r''_3 = r'_3 - \beta_0^2 \boldsymbol{\Delta_1} \\ = r_3 - \beta_0^2 d_2[1]^2 - \beta_1 d_2[1] - \beta_0 2 d_2[0] d_2[1] - \beta_0^2 \boldsymbol{\Delta_1}. \tag{6.1}$$

The optimization requirement, e.g., $r''_3 = 0$, leads to the expressions for Δ_1 and r''_4:

$$r''_3 = 0 \Rightarrow \Delta_1 = r'_3/\beta_0^2 \\ = r_3/\beta_0^2 - d_2[1]^2 - \beta_1/\beta_0^2 d_2[1] - 1/\beta_0 2 d_2[0] d_2[1], \tag{6.2a}$$

$$r''_4 = r'_4 - r'_3(\beta_1/\beta_0 + 2 d_2[0]). \tag{6.2b}$$

Numerical calculation at $n_f = 4$ gives the estimates for the values of the quantities in Eqs. (6.2a) and (6.2b),

$$r''_3 = 0, \qquad \Delta_1 \approx -3.7, \tag{6.3a}$$

$$r''_4 \approx -4740.52, \tag{6.3b}$$

$$a'_s \to a''_s = a_s(s \cdot e^{-0.692+3.7\beta_0 a'_s(s)}). \qquad (6.3c)$$

One may conclude that the PT expansion

$$R^{\rm NS} = 1 + 3C_{\rm F}\left\{a''_s + \frac{1}{3}\cdot(a''_s)^2 + 0\cdot(a''_s)^3 + r''_4\cdot(a''_s)^4 + \ldots\right\} \qquad (6.4)$$

significantly improves:

(i) $r'_3 = 0$, while the value of r''_4 in (6.5e) is less than in (5.11c) and (5.12c) and reduces twice in comparison with the PMC estimate in (5.13b) (taken for $n_f = 4$).

(ii) The domain of applicability of the approach extends to a wider region due to the opposite sign at Δ_1, compared to the one for PMC in (5.13a). This makes the NLO "shift" Δ less, which tends numerically to 0 at the boundary of applicability, $\Delta = d_2[1] + \Delta_1\beta_0 a'_s(s) \approx -0.692 + 3.7\beta_0 a'_s(s)$.

Indeed, following the usual PT condition $|d_2[1]| \gtrsim |\Delta_1\beta_0 a'_s(s)|$ or $\Delta \lesssim 0$, we get for the boundary $s \gtrsim 10$ GeV^2, as it is illustrated in Fig. 1 (left). The factor $\exp[-\Delta]$, entering in the argument of a''_s in Eq. (6.3c), see the solid (red) upper line in Fig. 1 (left), satisfies the conditions $1 \gtrsim \exp[-0.692 + 3.7\beta_0 a'_s(s)] > 1/2$, and this factor slowly decreases with s from the value 1. It looks tempting to get and use the exact solution for the coupling $a^\star_s$, following from Eq. (5.2),

$$a^\star_s(s) = a_s(s\exp[-\Delta_0 - \Delta_1\beta_0 a^\star_s(s)]),$$

rather than its iteration $a''_s(s)$. It is easy to obtain the useful inequality $a'_s(s) > a^\star_s(s) > a''_s(s)$; moreover, the numerical calculation gives that the difference between $a^\star_s$ and a''_s becomes noticeable below $s = 1$ GeV^2 for this optimized quantity and for the next one discussed below.

Similar optimization can be performed for $C^{\rm Bjp}_{\rm NS}(Q^2)$ ($n_f = 4$). We apply the general combined equations, analogous to the ones of Eqs. (5.3a)–(5.3d). In these $C^{\rm Bjp}_{\rm NS}$-oriented expressions we fix the conditions $c''_2 = 0$ and $c''_3 = 0$. This leads to the following equations:

$$c'_2 = 0, \qquad \Delta_0 = c_2/\beta_0 \approx 1.56,, \qquad (6.5a)$$

$$a_s \to a'_s = a_s(Q^2 \cdot e^{-1.56}) \qquad (6.5b)$$

$$c''_2 = c'_2 = 0, \qquad (6.5c)$$

$$c''_3 = 0, \qquad \Delta_1 \approx -0.396, \qquad (6.5d)$$

$$c''_4 \approx 4184.64, \qquad (6.5e)$$

$$a'_s \to a''_s = a_s(Q^2 \cdot e^{-1.56+0.396\beta_0 a'_s(Q^2)}). \qquad (6.5f)$$

The new "optimized scale" behavior of factor $\exp[-\Delta]$ is illustrated in Fig. 1 (right) by a solid (red) line, while the broken (blue) line there corresponds to the condition $c'_2 = 0, \Delta_0 = c_2/\beta_0$ that is not the BLM one. This transformation significantly improves the perturbative series for $C^{\rm Bjp}_{\rm NS}$,

$$C^{\rm Bjp}_{\rm NS}(Q^2) = 1 - 3C_{\rm F}\{a''_s + 0\cdot(a''_s)^2 + 0\cdot(a''_s)^3 + c''_4\cdot(a''_s)^4 + \ldots\}, \qquad (6.6)$$

in comparison with Eqs. (5.14a)–(5.14c), (5.15a)–(5.15c), and (5.16). We conclude that for both of the considered quantities the PT series are improved, and the corresponding Eqs. (6.3c) and (6.4) and Eqs. (6.5f) and (6.6) consist of the main results of this section. We did not perform the next step

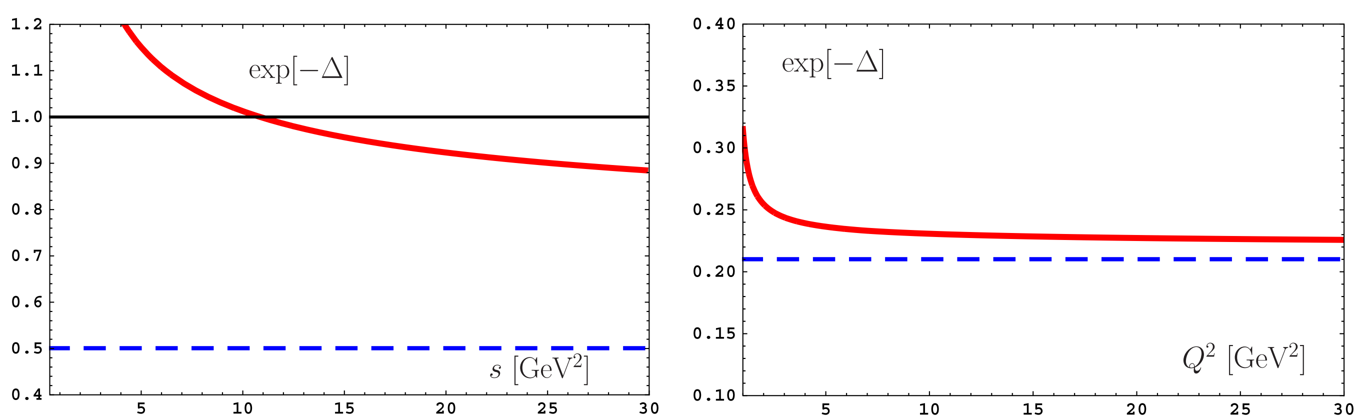

FIG. 1 (color online). Factors $\exp[-\Delta]$ at coupling scale: (Left) for $R^{\rm NS}(s)$. Solid (red) upper line—the NLO factor $\exp[-0.692 + 3.7\beta_0 a'_s(s)]$; long dashed (blue) line—the leading-order BLM one $\exp[-0.692]$. (Right) for $C^{\rm Bjp}_{\rm NS}(Q^2)$. Solid (red) upper line—the NLO factor $\exp[-1.56 + 0.396\beta_0 a'_s(Q^2)]$, long dashed (blue) line—the LO $\exp[-1.56]$.

of optimization with the coefficients r_4'', c_4'' because in this case we lost control under accuracy.

It is clear that Eqs. (6.5) and (6.4) and Eqs. (6.5a)–(6.5f) and (6.6) are not unique optimal solutions because different efficiency functions may be called "optimal." Therefore, one can satisfy one's own efficiency function with the coefficients $\{c_i\}$ based on the combined Eqs. (5.3a)–(5.3f) in the plane (Δ_0, Δ_1) or space $(\Delta_0, \Delta_1, \Delta_2, \ldots)$ of fitting free parameters Δ_j.

VII. CONCLUSION

We have considered the general structure of the perturbation expansion of renormalization group invariant quantities in MS schemes to clarify the effects of charge renormalization and the conformal symmetry breakdown. Following the line started in Ref. [8], we arrived at the matrix representation for this expansion, named the $\{\beta\}$ expansion [9], instead of the standard perturbation series. We discussed in great detail the unambiguity of this representation for the Adler $D^{\rm NS}$ function (or related $R_{e^+e^-}$ ratio) and for the Bjorken polarized sum rule $S^{\rm Bjp}$ (with the coefficient function $C^{\rm Bjp}_{\rm NS}$) for DIS in order $\mathcal{O}(\alpha_s^3)$. The expansion for $S^{\rm Bjp}$ was obtained by using different parts of the Crewther relation [9] for $D^{\rm NS}$ and the coefficient function $C^{\rm Bjp}_{\rm NS}$. Others attempts of this presentation [3–6] were discussed, too. We provided a new prediction for $C^{\rm Bjp}_{\rm NS}(a_s, n_f, n_{\tilde g})$ with the MSSM massless gluino $n_{\tilde g}$ in order $\mathcal{O}(\alpha_s^3)$ in Eqs. (4.11a)–(4.11c), Sec. IV B, as a byproduct of our consideration.

Based on the $\{\beta\}$ expansion, we constructed renormalization group transformation for the perturbation series of the considered quantities, Eqs. (5.3a)–(5.3f) in Sec. V. The initial expansion was split into two parts: a new series for the expansion coefficients and for the shift of the normalization scale of the coupling α_s. The contributions from each order can be balanced between these two series. Different procedures of the PT optimization, including PMC [4,5] and seBLM [8], were discussed and illustrated by numerical estimates. We conclude that the corrected PMC does not provide better PT series convergence and suggest our own scheme of the series optimization in order $\mathcal{O}(\alpha_s^4)$; the working formulas for $R^{\rm NS}$ of the $R_{e^+e^-}$ ratio and $C^{\rm Bjp}_{\rm NS}$ were presented in Sec. VI.

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APPENDIX A: EXPLICIT FORMULAS FOR $\beta(n_f, n_{\tilde g})$ AND $D(n_f, n_{\tilde g})$

The required β-function coefficients with the MSSM light gluinos [48] calculated in the $\overline{\rm MS}$ scheme are

$$\beta_0(n_f, n_{\tilde g}) = \frac{11}{3} C_A - \frac{4}{3}\left(T_R n_f + \frac{n_{\tilde g} C_A}{2}\right); \tag{A1a}$$

$$\beta_1(n_f, n_{\tilde g}) = \frac{34}{3} C_A^2 - \frac{20}{3} C_A \left(T_R n_f + \frac{n_{\tilde g} C_A}{2}\right) - 4\left(T_R n_f C_{\rm F} + \frac{n_{\tilde g} C_A}{2} C_A\right); \tag{A1b}$$

$$\beta_2(n_f, n_{\tilde g}) = \frac{2857}{54} C_A^3 - n_f T_R \left(\frac{1415}{27} C_A^2 + \frac{205}{9} C_A C_F - 2 C_F^2\right) + (n_f T_R)^2 \left(\frac{44}{9} C_F + \frac{158}{27} C_A\right) - \frac{988}{27} n_{\tilde g} C_A (C_A^2) + n_{\tilde g} C_A n_f T_R \left(\frac{22}{9} C_A C_F + \frac{224}{27} C_A^2\right) + (n_{\tilde g} C_A)^2 \frac{145}{54} C_A. \tag{A1c}$$

The β_3 coefficient, which includes the MSSM light gluinos, is not yet known, so we present it here in the standard [52,53] simplest form:

$$\beta_3(n_f) = C_A^4\left(\frac{150653}{486} - \frac{44}{9}\zeta_3\right) + C_A^3 T_R n_f\left(-\frac{39143}{81} + \frac{136}{3}\zeta_3\right) + C_F^2 T_R^2 n_f^2\left(\frac{1352}{27} - \frac{704}{9}\zeta_3\right)$$
$$+ C_A C_F T_R^2 n_f^2\left(\frac{17152}{243} + \frac{448}{9}\zeta_3\right) + C_A C_F^2 T_R n_f\left(-\frac{4204}{27} + \frac{352}{9}\zeta_3\right) + \frac{424}{243} C_A T_R^3 n_f^3$$
$$+ C_A^2 C_F T_R n_f\left(\frac{7073}{243} - \frac{656}{9}\zeta_3\right) + C_A^2 T_R^2 n_f^2\left(\frac{7930}{81} + \frac{224}{9}\zeta_3\right) + \frac{1232}{243} C_F T_R^3 n_f^3 + 46 C_F^3 T_R n_f$$
$$+ n_f \frac{d_F^{abcd} d_A^{abcd}}{N_A}\left(\frac{512}{9} - \frac{1664}{3}\zeta_3\right) + n_f^2 \frac{d_F^{abcd} d_F^{abcd}}{N_A}\left(-\frac{704}{9} + \frac{512}{3}\zeta_3\right) + \frac{d_A^{abcd} d_A^{abcd}}{N_A}\left(-\frac{80}{9} + \frac{704}{3}\zeta_3\right). \quad \text{(A2)}$$

For the $SU_c(N)$ color group with fundamental fermions, the invariants read

$$T_R = \frac{1}{2}, \qquad C_F = \frac{N^2-1}{2N}, \qquad C_A = N, \qquad d^{abc}d^{abc} = \frac{(N^2-4)N_A}{N}; \qquad N_A = 2C_F C_A \equiv N^2 - 1. \quad \text{(A3)}$$

$$\frac{d_F^{abcd} d_A^{abcd}}{N_A} = \frac{N(N^2+6)}{48}, \qquad \frac{d_A^{abcd} d_A^{abcd}}{N_A} = \frac{N^2(N^2+36)}{24}, \qquad \frac{d_F^{abcd} d_F^{abcd}}{N_A} = \frac{N^4 - 6N^2 + 18}{96N^2}. \quad \text{(A4)}$$

The $D^{\rm NS}$ function evaluated in Ref. [25] in the same model in the case in which the masses of gluions are neglected[5] reads

$$D^{\rm NS}(a_s, n_f, n_{\tilde g}) = 1 + a_s \cdot (3C_F) \quad \text{(A5a)}$$

$$+ a_s^2\left\{-\frac{3}{2}C_F^2 + 2C_F\left[\frac{123}{2} - 44\zeta_3 - (11 - 8\zeta_3)n_{\tilde g}\right]\frac{C_A}{2} - 2C_F(11 - 8\zeta_3)n_f T_R\right\} \quad \text{(A5b)}$$

$$+ a_s^3\left\{-\frac{69}{2}C_F^3 - C_F^2 C_A[127 + 572\zeta_3 - 880\zeta_5 - (36 + 104\zeta_3 - 160\zeta_5)n_{\tilde g}]\right.$$
$$+ C_F C_A^2\left[\frac{90445}{54} - \frac{10948}{9}\zeta_3 - \frac{440}{3}\zeta_5 - \left(\frac{33767}{54} - \frac{4016}{9}\zeta_3 - \frac{80}{3}\zeta_5\right)n_{\tilde g}\right.$$
$$\left. + \left(\frac{1208}{27} - \frac{304}{9}\zeta_3\right)n_{\tilde g}^2\right] - n_f T_R C_F^2[29 - 304\zeta_3 + 320\zeta_5]$$
$$- n_f T_R C_F C_A\left[\frac{31040}{27} - \frac{7168}{9}\zeta_3 - \frac{160}{3}\zeta_5 - \left(\frac{4832}{27} - \frac{1216}{9}\zeta_3\right)n_{\tilde g}\right]$$
$$\left. + 3C_F\left[\frac{302}{9} - \frac{76}{3}\zeta_3\right]\left(\frac{4}{3}T_R n_f\right)^2\right\} = \quad \text{(A5c)}$$

$$= 1 + a_s(3C_F) + a_s^2(3C_F)\cdot\left\{\frac{C_A}{3} - \frac{C_F}{2} + \left(\frac{11}{2} - 4\zeta_3\right)\beta_0(n_f, n_{\tilde g})\right\}$$
$$+ a_s^3(3C_F)\cdot\left\{\left(\frac{302}{9} - \frac{76}{3}\zeta_3\right)\beta_0^2(n_f, n_{\tilde g}) + \left(\frac{101}{12} - 8\zeta_3\right)\beta_1(n_f, n_{\tilde g})\right.$$
$$+ \left[C_A\left(\frac{3}{4} + \frac{80}{3}\zeta_3 - \frac{40}{3}\zeta_5\right) - C_F(18 + 52\zeta_3 - 80\zeta_5)\right]\beta_0(n_f, n_{\tilde g}) \quad \text{(A6a)}$$

$$\left. + \left(\frac{523}{36} - 72\zeta_3\right)C_A^2 + \frac{71}{3}C_A C_F - \frac{23}{2}C_F^2\right\}. \quad \text{(A6b)}$$

[5]In the numerical case, this expression from Ref. [25] coincides with the result of the related numerical calculation of Ref. [54].

The Bjorken coefficient function $C_{\rm NS}^{\rm Bjp}$ of the DIS sum rules calculated first in Ref. [38] is

$$C_{\rm NS}^{\rm Bjp}(a_s, n_f) = 1 + a_s(-3C_F) \tag{A7a}$$

$$+a_s^2(-3C_F)\left[-\frac{7}{2}C_F + \frac{23}{3}C_A - \frac{8}{3}T_R n_f\right] \tag{A7b}$$

$$+ a_s^3(-3C_F)\left\{\frac{C_F^2}{2} + C_F C_A\left[\frac{176}{9}\zeta_3 - \frac{1241}{27}\right] + C_A^2\left[\frac{10874}{81} - \frac{440}{9}\zeta_5\right]\right. \tag{A7c}$$

$$\left.+n_f T_R C_F\left[\frac{133}{27} - \frac{80}{9}\zeta_3\right] - n_f T_R C_A\left[\frac{7070}{81} + 16\zeta_3 - \frac{160}{9}\zeta_5\right] + \frac{115}{18}\left(\frac{4}{3}n_f T_R\right)^2\right\}. \tag{A7d}$$

The prediction for C_{Bjp} obtained in Sec. IV B of this article under the same conditions as Eq. (A5a)–(A5c) reads

$$C_{\rm NS}^{\rm Bjp}(a_s, n_f, n_{\tilde{g}}) = 1 + a_s(-3C_F) \tag{A8a}$$

$$+ a_s^2(-3C_F)\cdot\left\{\frac{1}{3}C_A - \frac{7}{2}C_F + 2\beta_0(n_f, n_{\tilde{g}})\right\} \tag{A8b}$$

$$+ a_s^3(-3C_F)\cdot\left\{\frac{115}{18}\beta_0^2(n_f, n_{\tilde{g}}) + \left(\frac{59}{12} - 4\zeta_3\right)\beta_1(n_f, n_{\tilde{g}})\right.$$
$$\left.-\left[\left(\frac{215}{36} - 32\zeta_3 + \frac{40}{3}\zeta_5\right)C_A + \left(\frac{166}{9} - \frac{16}{3}\zeta_3\right)C_F\right]\beta_0(n_f, n_{\tilde{g}}) + \left(\frac{523}{36} - 72\zeta_3\right)C_A^2 + \frac{65}{3}C_F C_A + \frac{C_F^2}{2}\right\}. \tag{A8c}$$

APPENDIX B: NATURAL FORMS FOR β EXPANSION OF $D^{\rm NS}$ AND $C^{\rm NS}$

Here, we present for completeness the results of (4.8a)–(4.8e) and (4.10a)–(4.10e) in their natural form, changing only the normalization factors [9], which correspond to the coupling $\frac{\alpha_s}{\pi}$ with $\beta_0 = \frac{1}{4}(\frac{11}{3}C_A - \frac{4}{3}(T_R n_f + n_{\tilde{g}}C_A\frac{1}{2})), \ldots,$

$$d_1^{\rm NS} = \frac{3}{4}C_F, \tag{B1a}$$

$$d_2^{\rm NS}[1] = \left(\frac{33}{8} - 3\zeta_3\right)C_F, \qquad d_2^{\rm NS}[0] = -\frac{3}{32}C_F^2 + \frac{1}{16}C_F C_A, \tag{B1b}$$

$$d_3^{\rm NS}[2] = \left(\frac{151}{6} - 19\zeta_3\right)C_F, \qquad d_3^{\rm NS}[0,1] = \left(\frac{101}{16} - 6\zeta_3\right)C_F, \tag{B1c}$$

$$d_3^{\rm NS}[1] = \left(-\frac{27}{8} - \frac{39}{4}\zeta_3 + 15\zeta_5\right)C_F^2 - \left(\frac{9}{64} - 5\zeta_3 + \frac{5}{2}\zeta_5\right)C_F C_A, \tag{B1d}$$

$$d_3[0] = -\frac{69}{128}C_F^3 + \frac{71}{64}C_F^2 C_A + \left(\frac{523}{768} - \frac{27}{8}\zeta_3\right)C_F C_A^2; \tag{B1e}$$

$$c_1^{\rm NS} = -\frac{3}{4}C_F, \tag{B2a}$$

$$c_2^{\rm NS}[1] = -\frac{3}{2}C_F, \qquad c_2^{\rm NS}[0] = \frac{21}{32}C_F^2 - \frac{1}{16}C_F C_A, \tag{B2b}$$

$$c_3^{\rm NS}[2] = -\frac{115}{24}\mathrm{C_F}, \qquad c_3^{\rm NS}[1] = \left(\frac{83}{24} - \zeta_3\right)\mathrm{C_F^2} + \left(\frac{215}{192} - 6\zeta_3 + \frac{5}{2}\zeta_5\right)\mathrm{C_F}C_A, \tag{B2c}$$

$$c_3^{\rm NS}[0,1] = \left(-\frac{59}{16} + 3\zeta_3\right)\mathrm{C_F}, \tag{B2d}$$

$$c_3^{\rm NS}[0] = -\frac{3}{128}\mathrm{C_F^3} - \frac{65}{64}\mathrm{C_F^2}C_A - \left(\frac{523}{768} - \frac{27}{8}\zeta_3\right)\mathrm{C_F}C_A^2. \tag{B2e}$$

APPENDIX C: EXPLICIT FORMULAS FOR Δ_i

The explicit expressions for the elements of the proper scales Δ_1 and Δ_2 are given by

$$\Delta_0 = d_2[1]; \tag{C1}$$

$$\Delta_1 = d_3[2] - d_2^2[1] - \pi^2/3 + \frac{\beta_1}{\beta_0^2}(d_3[0,1] - d_2[1]) + \frac{1}{\beta_0}\underline{\underline{(d_3[1] - 2d_2[1]d_2[0])}}; \tag{C2}$$

$$\begin{aligned}\Delta_2 = {} & (d_4[3] - 3d_2[1]d_3[2] + 2(d_2[1])^3 - \pi^2 d_2[1]) + \beta_2/\beta_0^3(d_4[0,0,1] - d_2[1]) \\ & + \beta_1/\beta_0^2[d_4[1,1] - 3d_3[0,1]d_2[1] + \frac{3}{2}(d_2[1])^2 - d_3[2] - \pi^2/2] \\ & + \beta_1^2/\beta_0^4(d_2[1] - d_3[0,1]) + \beta_1/\beta_0^3\underline{\underline{(d_4[0,1] - d_3[1] - 2d_2[0](d_3[0,1] - d_2[1]))}} +\end{aligned} \tag{C3}$$

$$1/\beta_0\underline{\underline{[d_4[2] - 3d_3[1]d_2[1] + d_2[0](5d_2[1]^2 - 2d_3[2] - \pi^2/3)]}} + \tag{C4}$$

$$1/\beta_0^2\underline{\underline{[d_4[1] - 3d_3[0]d_2[1] + 2d_2[0](2d_2[1]d_2[0] - d_3[1])]}}. \tag{C5}$$

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