

Scale- and scheme-independent extension of Padé approximants: Bjorken polarized sum rule as an example

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A renormalization-scale-invariant generalization of the diagonal Padé approximants (DPA), developed previously, is extended so that it becomes renormalization-scheme invariant as well. We do this explicitly when two terms beyond the leading order (NNLO, $\sim \alpha_s^3$) are known in the truncated perturbation series (TPS). At first, the scheme dependence shows up as a dependence on the first two scheme parameters c_2 and c_3 . Invariance under the change of the leading parameter c_2 is achieved via a variant of the principle of minimal sensitivity. The subleading parameter c_3 is fixed so that a scale- and scheme-invariant Borel transform of the resummation approximant gives the correct location of the leading infrared renormalon pole. The leading higher-twist contribution, or a part of it, is thus believed to be contained implicitly in the resummation. We applied the approximant to the Bjorken polarized sum rule (BPSR) at $Q_{\text{ph}}^2 = 5$ and 3 GeV^2 , for the most recent data and the data available until 1997, respectively, and obtained $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.119_{-0.006}^{+0.003}$ and $0.113_{-0.019}^{+0.004}$, respectively. Very similar results are obtained with Grunberg's effective charge method and Stevenson's TPS principle of minimal sensitivity, if we fix the c_3 parameter in them by the aforementioned procedure. The central values for $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ increase to 0.120 (0.114) when applying DPA's, and 0.125 (0.118) when applying NNLO TPS.

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I. INTRODUCTION

The problem of extracting as much information as possible from an available QCD or QED truncated perturbation series (TPS) of an observable, and including this information in a resummed result, was the focus of several works during the last twenty years. Most of these resummation methods are based on the available TPS only. Some of these latter methods eliminate the unphysical dependence of the TPS on the renormalization scale (RScI) and scheme (RSch) by fixing them in the TPS itself. Among these methods are the Brodsky-Lepage-Mackenzie (BLM) fixing motivated by large- n_f considerations [1], the principle of minimal sensitivity (PMS) [2], and the effective charge method (ECH) [3,4] (see Ref. [5] for a related method). Some of the more recent approaches in this direction include approaches related with the method of "commensurate scale relations" [6], an approach using an analytic form of the coupling parameter [7], ECH-related approaches [8], a method using expansions in the two-loop coupling parameter [9] expressed in terms of the Lambert function [10], and methods using conformal transformations either for the Borel expansion parameter [11] or for the coupling parameter [12]. A basically different method consists in replacing the TPS by Padé approximants

(PA's) which provide a resummation of the TPS such that the resummed results show weakened RScI- and RSch-dependence [13]. In particular, the diagonal Padé approximants (DPA's) were shown to be particularly well motivated since they are RScI independent in the approximation of the one-loop evolution of the coupling $\alpha_s(Q^2)$ [14]. An additional advantage of PA's is connected with the fact that they surmount the purely polynomial structure of the TPS's on which they are based, and thus offer a possibility of accounting for at least some of the nonperturbative contributions, via a strong mechanism of quasianalytic continuation implicitly contained in PA's.

Recently, we proposed a generalization of the method of DPA's which achieves the exact perturbative RScI independence of the resummed result [15]. While this procedure in its original form was restricted to the cases where the number of available TPS terms beyond the leading order [(LO): $\sim \alpha^1$] is odd, it was subsequently extended to the remaining cases where this number is even [16]. This would then apply to those QCD observables where the number of such known terms is 2 (NNLO, $\sim \alpha_s^3$).¹ In Ref. [16] we also speculated on ways how to eliminate the leading RSch dependence from our approximants A , and proposed for the NNLO case a simple way following the principle of minimal sensitivity (PMS). It turns out that the way proposed there does not

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¹When just one such term is known (NLO), our approximants give the same result as the ECH method.

work properly in practice since no minimum of the PMS equation $\partial A/\partial c_2=0$ [see Eq. (40) there] can be found. The dependence of our approximants on the RSch parameters $c_2\equiv\beta_2/\beta_0$ and $c_3\equiv\beta_3/\beta_0$ of the original TPS is definitely a problem when the approximants are applied to the low-energy observables such as the Bjorken polarized sum rule (BPSR) at the low momentum transfer of the virtual photon, e.g., $Q_{\text{ph}}^2\approx 3-5\text{ GeV}^2$ [17].

In the present work, we address this problem. For the NNLO TPS case, we construct in Sec. II an extended version \mathcal{A} of our approximants, in which the dependence on the leading RSch parameter c_2 is successfully eliminated by application of a variant of PMS conditions $\partial\mathcal{A}/\partial c_2^{(j)}=0$. This procedure can be extended in a straightforward way to the cases where more terms are known in the TPS, e.g., the NNNLO cases available now in QED, but we will not discuss such cases here. In Sec. III, we apply our approximant to the BPSR at such Q_{ph}^2 where three quark flavors are assumed active, e.g., $Q_{\text{ph}}^2\approx 3-5\text{ GeV}^2$. While the approximant at this stage is an RScl-independent and c_2 -independent generalization of the diagonal Padé approximant (DPA) [2/2], it still contains c_3 dependence comparable to that of the ECH [3] and TPS-PMS [2] methods. Subsequently, we fix the value of c_3 in our, the ECH, and the TPS-PMS approximants so that PA's of a modified (RScl- and RSch-independent) Borel transform of these approximants yield the correct location of the leading infrared (IR) renormalon pole. Thus, in the approximants we implicitly use β functions which go beyond the last perturbatively calculated order of the observable (NNLO), in order to incorporate the aforementioned nonperturbative information. In Sec. IV we then compare the values of these resummation approximants with the values for the BPSR extracted from experiments, and obtain predictions for $\alpha_s(M_Z^2)$. We also apply the TPS and various PA methods of resummation to these values of the BPSR and obtain higher values for $\alpha_s(M_Z^2)$. In Sec. V we redo the calculations by applying a PA-type quasianalytic continuation for the β functions relevant for our, ECH, and TPS-PMS approximants. We further address the question of higher-twist terms. In Sec. VI we discuss the obtained numerical results for $\alpha_s(M_Z^2)$ and Sec. VII contains a summary and outlook.

A brief version containing a summarized description and application of the method can be found in Ref. [18]. In contrast to Ref. [18], the numerical analysis of the BPSR in the present paper (Secs. IV, V) uses, in addition, the most recent data of the E155 Collaboration [19].

II. CONSTRUCTION OF c_2 -INDEPENDENT APPROXIMANTS

Let us consider a (QCD) observable S , with negligible mass effects, which is normalized so that its perturbative expansion takes the canonical form

$$S=a_0(1+r_1a_0+r_2a_0^2+r_3a_0^3+\dots), \quad (1)$$

where $a_0\equiv\alpha_s^{(0)}/\pi$. We suppose that this expansion is calculated within a specific RSch and using a specific (Euclidean)

RScl Q_0 (symbol “0” is generically attached to the RScl and RSch parameters in the TPS) up to NNLO, yielding as the result the TPS

$$S_{[2]}=a_0(1+r_1a_0+r_2a_0^2). \quad (2)$$

Here, both a_0 and the coefficients r_1 and r_2 are RScl and RSch dependent. The coupling parameter $a\equiv\alpha_s/\pi$ evolves under the change of the energy scale (RScl) Q , within the given RSch, according to the following renormalization group equation (RGE):

$$\frac{\partial a(\ln Q^2; c_2^{(0)}, \dots)}{\partial \ln(Q^2)} = -\beta_0 a^2(1+c_1a+c_2^{(0)}a^2+c_3^{(0)}a^3+\dots), \quad (3)$$

where β_0 and c_1 are universal quantities (RScl and RSch invariant),² whereas the remaining coefficients $c_j^{(0)}$ ($j\geq 2$) are RSch dependent and their values can—on the other hand—be used to characterize the RSch. Consequently, in Eq. (2) the coupling parameter a_0 is a function of the RScl and RSch

$$a_0\equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots). \quad (4)$$

The NLO and NNLO coefficients in Eq. (2) have, due to the RScl and RSch independence of S , the following RScl and RSch dependence:

$$\begin{aligned} r_1 &\equiv r_1(\ln Q_0^2) = r_1(\ln \tilde{Q}^2) + \beta_0 \ln(Q_0^2/\tilde{Q}^2), \\ r_2 &\equiv r_2(\ln Q_0^2; c_2^{(0)}) = r_1^2(\ln Q_0^2) + c_1 r_1(\ln Q_0^2) - c_2^{(0)} + \rho_2, \end{aligned} \quad (5)$$

where ρ_2 is RScl and RSch invariant. Although the physical quantity S must be independent of the RScl and RSch, its TPS (2) possesses an unphysical dependence on RScl and RSch which manifests itself in higher order terms

$$\frac{\partial S_{[2]}}{\partial \ln Q_0^2} \sim a_0^4 \sim \frac{\partial S_{[2]}}{\partial c_2^{(0)}} \sim \frac{\partial S_{[2]}}{\partial c_3^{(0)}}. \quad (6)$$

All approximants to S which are based on TPS (2) must fulfill the minimal condition: when expanded in powers of a_0 to order a_0^3 , they must reproduce TPS (2). Further, since the full S is RScl and RSch independent, the approximant should preferably share this property with S if it is to bring us closer to the actual value of S . The generalization of the diagonal Padé approximants developed in Ref. [15] possesses full RScl independence for massless observables.

In its original form it is accountable only to TPS with an odd number of terms beyond the leading order (LO: $\sim a^1$). Unfortunately, however, QCD observables have been calculated at most to the NNLO, i.e., at best the TPS (2) is known.

² $\beta_0=(11-2n_f/3)/4$, $c_1=(102-38n_f/3)/(16\beta_0)$, where n_f is the number of active quark flavors.

Therefore, in Ref. [16] we have extended the method to the cases with even numbers of terms beyond the LO, in particular for the TPS of the type (2). Since within the present paper we are going to apply an extended related procedure to these cases of $S_{[2]}$, we recapitulate briefly the main steps for treating a TPS of the generic form $S_{[2]}$. The trick consisted in introducing—in addition to S —the auxiliary observable $\tilde{S} \equiv S^*S$, which then gets the following formal canonical form:

$$\tilde{S} = (S)^2 = a_0(0 + a_0 + R_2 a_0^2 + R_3 a_0^3 + \dots), \quad (7)$$

where

$$R_2 = 2r_1, \quad R_3 = r_1^2 + 2r_2, \dots, \quad (8)$$

\tilde{S} is then known formally to NNNLO ($\sim a^4$) and the method can thus be applied, yielding an approximant $\mathcal{A}_{S^2}^{[2/2]}$ to \tilde{S} . The corresponding approximant to S is $\sqrt{\mathcal{A}_{S^2}^{[2/2]}}$ which has the form [16]

$$\begin{aligned} \sqrt{\mathcal{A}_{\tilde{S}}^{[2/2]}} &= \{\tilde{\alpha}_0 [a(\ln \tilde{Q}_1^2; c_2^{(0)}, c_3^{(0)}, \dots) \\ &\quad - a(\ln \tilde{Q}_2^2; c_2^{(0)}, c_3^{(0)}, \dots)]\}^{1/2} \\ &= [S_{[2]} + \mathcal{O}(a^4)], \end{aligned} \quad (9)$$

and it is again exactly RScl invariant. Here, the two scales \tilde{Q}_j ($j=1,2$) and the factor $\tilde{\alpha}_0$ are independent of the RScl Q_0 and determined by the identities

$$\left(\frac{\ln(\tilde{Q}_2^2/Q_0^2)}{\ln(\tilde{Q}_1^2/Q_0^2)} \right) = \frac{1}{2\beta_0} [\tilde{b}_1 \pm \sqrt{\tilde{b}_1^2 - 4\tilde{b}_2}], \quad \tilde{\alpha}_0 = \frac{1}{\sqrt{\tilde{b}_1^2 - 4\tilde{b}_2}}, \quad (10)$$

$$\tilde{b}_1 = c_1 - 2r_1,$$

$$\tilde{b}_2 = -\frac{3}{2}c_1^2 + c_2^{(0)} + c_1 r_1 + 3r_1^2 - 2r_2. \quad (11)$$

If we ignore all higher than one-loop evolution effects, i.e., if we set $c_1 = 0 = c_2^{(0)}$ in Eqs. (10),(11) and replace the two coupling parameters in Eq. (9) by their one-loop evolved (from RScl Q_0^2 to \tilde{Q}_j^2) counterparts, then the approximant (9) becomes the square root of the [2/2] Padé approximant of \tilde{S} . This follows from general considerations in Refs. [15,16], but can also be verified directly in this special case. The approximant $[2/2]_{\tilde{S}}^{1/2}$ preserves the RScl invariance only approximately [in the one-loop renormalization group equation (RGE) approximation].

Although the RScl dependence is eliminated completely by using the approximant (9), there remains a RSch dependence, i.e., dependence on $c_j^{(0)}$ ($j \geq 2$). It manifests itself to a large degree due to $\partial \tilde{b}_2 / \partial c_2^{(0)} \neq 0$ ($\partial \tilde{b}_2 / \partial c_2^{(0)} = 3$). In Ref. [16] we speculated that the dependence on the leading RSch parameter $c_2^{(0)}$ could be eliminated by imposing the PMS condition of local independence [see Eq. (40) in Ref. [16]]

$$\left. \frac{d\mathcal{A}_{\tilde{S}}^{[2/2]}(\{\ln \tilde{Q}_j^2(c_2^{(0)})\}_{j=2,3,\dots})}{dc_2^{(0)}} \right|_{c_3^{(0)}, \dots} = 0, \quad (12)$$

where implicitly “=0” should be understood as “ $\sim a_0^6$ ” since in general this derivative is $\sim a_0^5$. However, expansion of this expression in powers of the coupling a_0 (or any a) yields

$$\left. \frac{d\mathcal{A}_{\tilde{S}}^{[2/2]}}{dc_2^{(0)}} \right|_{c_3^{(0)}, \dots} = -10c_1 a_0^5 + \mathcal{O}(a_0^6). \quad (13)$$

This implies that the approximant (9) to S has no stationary (PMS) point with respect to the RSch parameter $c_2^{(0)}$, since the coefficient of the leading term in the expansion of the derivative is constant and cannot be made equal to zero by a change of the RSch. Also actual numerical calculations for various observables S confirm this.

Therefore, we will modify the approximant (9) so that the new one will allow us to remove, by a PMS condition, the dependence on the leading RSch parameter $c_2^{(0)}$. This modification must, of course, be such that the aforementioned minimal condition is satisfied and that the RScl invariance is preserved. We do this in the following way. We keep the overall functional structure of Eq. (9). However, we replace the single set of RSch parameters $c_j^{(0)}$ ($j \geq 2$), which we inherited from the TPS, by two sets of a priori arbitrary parameters $c_j^{(1)}$ and $c_j^{(2)}$ ($j \geq 2$) in the two coupling parameters, respectively, and we also admit new values of the reference momenta Q_1^2 and Q_2^2

$$\begin{aligned} \sqrt{\mathcal{A}_{\tilde{S}}^{[2/2]}} &= \{\tilde{\alpha} [a(\ln Q_1^2; c_2^{(1)}, c_3^{(1)}, \dots) \\ &\quad - a(\ln Q_2^2; c_2^{(2)}, c_3^{(2)}, \dots)]\}^{1/2} \\ &= [S_{[2]} + \mathcal{O}(a^4)]. \end{aligned} \quad (14)$$

The parameters $c_j^{(1)}$ and $c_j^{(2)}$ will be appropriately fixed. They will turn out to be independent of the RSch parameters $c_j^{(0)}$ and of the RScl Q_0^2 of the original TPS, just like the scales Q_1^2 and Q_2^2 and the parameter $\tilde{\alpha}$ will be.³ We will now require $c_2^{(1)} \neq c_2^{(2)}$, in contrast to Eq. (9) which led us to the problem (13). This requirement is not unnatural, since the forms (9) and (14) have $\tilde{Q}_1^2 \neq \tilde{Q}_2^2$ and $Q_1^2 \neq Q_2^2$, respectively. The two new momentum scales Q_j and the parameter $\tilde{\alpha}$ in Eq. (14) will be determined, in terms of $c_k^{(j)}$'s ($k=2,3$; $j=1,2$), by expanding the two coupling parameters in power series of the original coupling a_0 (4) and requiring that the minimal condition be fulfilled, i.e., that the power series for $\mathcal{A}_{S^2}^{[2/2]}$ coincides with that of \tilde{S} (7),(8) up to (and including)

³Parameters $c_2^{(1)}$ and $c_2^{(2)}$ will be chosen later in the section, by following a variant of the PMS; $c_3^{(1)}$ and $c_3^{(2)}$ will be set equal to each other and fixed in the next sections.

$\sim a_0^4$. For this purpose we use the expansion for the general $a \equiv a(\ln Q^2; c_2, c_3, \dots)$ in powers of $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots)$ as obtained in Appendix A [Eqs. (A7)–(A9)], and apply it to as yet unspecified parameters Q_1^2 , Q_2^2 , and $c_k^{(j)}$ ($j=1,2$). The resulting expressions, when introduced into the square of the right-hand side of Eq. (14), yield an expansion in powers of a_0 . According to the minimal condition, it should coincide with Eq. (7) up to $\sim a_0^4$. Comparison of the coefficients of a_0^n ($n=2,3,4$) leads to the following relations:

$$\begin{aligned} \text{at } a_0^2: \quad & 1 = -\tilde{\alpha}(x_1 - x_2), \\ \Rightarrow \tilde{\alpha} &= \frac{(-1)}{(x_1 - x_2)} = \frac{(-1)}{\beta_0 \ln(Q_1^2/Q_2^2)}, \end{aligned} \quad (15)$$

$$\begin{aligned} \text{at } a_0^3: \quad & 2r_1 = -[(x_1^2 - x_2^2) - c_1(x_1 - x_2) \\ & + \delta c_2]/(x_1 - x_2), \end{aligned} \quad (16)$$

$$\begin{aligned} \text{at } a_0^4: \quad & 2r_2 + r_1^2 = -\left[-(x_1^3 - x_2^3) + \frac{5}{2}c_1(x_1^2 - x_2^2) \right. \\ & \left. - c_2^{(0)}(x_1 - x_2) - 3(x_1 \delta c_2^{(1)} - x_2 \delta c_2^{(2)}) \right. \\ & \left. + \frac{1}{2} \delta c_3 \right] / (x_1 - x_2), \end{aligned} \quad (17)$$

where we have used the notations

$$x_j \equiv \beta_0 \ln(Q_j^2/Q_0^2), \quad \delta c_2^{(j)} \equiv c_2^{(j)} - c_2^{(0)} \quad (j=1,2), \quad (18)$$

$$\delta c_2 \equiv c_2^{(1)} - c_2^{(2)}, \quad \delta c_3 \equiv c_3^{(1)} - c_3^{(2)}. \quad (19)$$

Equations (16) and (17) are the two equations which determine the two scales Q_1 and Q_2 (\Leftrightarrow parameters x_1 and x_2) as functions of $c_k^{(j)}$'s ($k=2,3$; $j=1,2$). In order to see that these two scales are independent of the original RScl (Q_0) and of the original RSch ($c_k^{(0)}$, $k \geq 2$), we introduce

$$\tilde{x}_j \equiv \beta_0 \ln(Q_j^2/\tilde{\Lambda}^2) \quad (j=1,2), \quad (20)$$

where $\tilde{\Lambda}$ is the universal QCD scale appearing in the Stevenson equation (A1), so it is RScl and RSch invariant. After some algebra, we can rewrite Eqs. (16) and (17) as a system of equations for \tilde{x}_j

$$2\rho_1 + c_1 = (\tilde{x}_1 + \tilde{x}_2) + \frac{\delta c_2}{(\tilde{x}_1 - \tilde{x}_2)}, \quad (21)$$

$$\begin{aligned} 2\rho_2 + 3\rho_1^2 - 2c_1\rho_1 &= (\tilde{x}_1^2 + \tilde{x}_1\tilde{x}_2 + \tilde{x}_2^2) - \frac{5}{2}c_1(\tilde{x}_1 + \tilde{x}_2) \\ &+ 3\frac{(\tilde{x}_1 c_2^{(1)} - \tilde{x}_2 c_2^{(2)})}{(\tilde{x}_1 - \tilde{x}_2)} - \frac{\delta c_3}{2(\tilde{x}_1 - \tilde{x}_2)}, \end{aligned} \quad (22)$$

where ρ_1 and ρ_2 are the usual RScl and RSch invariants as defined, e.g., in Ref. [2]⁴ [see also Eq. (5)]

$$\rho_1 = \beta_0 \ln(Q_0^2/\tilde{\Lambda}^2) - r_1, \quad (23)$$

$$\rho_2 = r_2 - r_1^2 - c_1 r_1 + c_2^{(0)}. \quad (24)$$

Therefore, Eqs. (21),(22) show the following: If $c_2^{(1)}$ and $c_2^{(2)}$ and $\delta c_3 \equiv c_3^{(1)} - c_3^{(2)}$ are chosen and fixed, then the solutions \tilde{x}_j and thus the scales Q_j ($j=1,2$) are independent of the RScl (Q_0) and of the RSch ($c_2^{(0)}, c_3^{(0)}, \dots$). Thus, we have

$$\begin{aligned} Q_j^2 &= Q_j^2(c_2^{(1)}, c_2^{(2)}; \delta c_3) \quad (j=1,2), \\ \tilde{\alpha} &= \frac{(-1)}{\beta_0 \ln(Q_1^2/Q_2^2)} = \tilde{\alpha}(c_2^{(1)}, c_2^{(2)}; \delta c_3). \end{aligned} \quad (25)$$

Therefore, our approximant (14) will be regarded from now on as a function of only $c_k^{(j)}$ parameters ($k \geq 2$; $j=1,2$): $\mathcal{A}_{S^2}^{[2/2]}(c_2^{(1)}, c_2^{(2)}; c_3^{(1)}, c_3^{(2)}; \dots)$. For actually solving the equations for the scales Q_1 and Q_2 , it is more convenient to use Eqs. (16),(17). For the subsequent use, we rewrite them in the following form:

$$y_-^4 - y_-^2 z_0^2(c_2^{(s)}) + y_- \frac{1}{4}(5c_1 \delta c_2 - \delta c_3) - \frac{3}{16}(\delta c_2)^2 = 0, \quad (26)$$

$$-r_1 + \frac{1}{2}c_1 - \frac{1}{4}\frac{\delta c_2}{y_-} = y_+, \quad (27)$$

where we use the notations

$$y_{\pm} \equiv \frac{1}{2}\beta_0 \left[\ln \frac{Q_1^2}{Q_0^2} \pm \ln \frac{Q_2^2}{Q_0^2} \right], \quad (28)$$

$$\delta c_k \equiv c_k^{(1)} - c_k^{(2)}, \quad c_k^{(s)} \equiv \frac{1}{2}(c_k^{(1)} + c_k^{(2)}) \quad (k=2,3), \quad (29)$$

$$z_0^2 \equiv \left(2\rho_2 + \frac{7}{4}c_1^2 \right) - 3c_2^{(s)} \equiv z_0^2(c_2^{(s)}), \quad (30)$$

where ρ_2 is given by Eq. (24). Incidentally, it can be explicitly checked that in the special case of $c_2^{(1)} = c_2^{(2)} = c_2^{(0)}$ and $c_3^{(1)} = c_3^{(2)} = c_3^{(0)}$ Eqs. (26)–(30) and (16) recover the old approximant (9)–(11) of Ref. [16].

The next question is how to fix parameters $c_2^{(j)}$ and $c_3^{(j)}$ ($j=1,2$). Above all, we have to fix the leading parameters $c_2^{(j)}$'s since otherwise their arbitrariness would reflect the fact

⁴Rączka [20] used the sum of the absolute values of terms in ρ_2 for a formulation of criteria for acceptable RScl's and RSch's in NNLO TPS. He concluded that the strong RScl/RSch dependence of the NNLO TPS of the BjPSR (with $n_f=3$) presents a serious practical problem.

that the leading RSch dependence (i.e., the dependence on $c_2^{(0)}$) has not been eliminated from the approximant. We do this by requiring the local independence of the approximant with respect to variation of $c_2^{(1)}$ and of $c_2^{(2)}$ separately. This condition is a variant of the principle of minimal sensitivity (PMS), or a PMS-type ansatz

$$\left. \frac{\partial \mathcal{A}_{\bar{s}}^{[2/2]}}{\partial c_2^{(1)}} \right|_{c_2^{(2)}} = 0 = \left. \frac{\partial \mathcal{A}_{\bar{s}}^{[2/2]}}{\partial c_2^{(2)}} \right|_{c_2^{(1)}} \Leftrightarrow \left. \frac{\partial \mathcal{A}_{\bar{s}}^{[2/2]}}{\partial c_2^{(s)}} \right|_{\delta c_2} = 0 = \left. \frac{\partial \mathcal{A}_{\bar{s}}^{[2/2]}}{\partial (\delta c_2)} \right|_{c_2^{(s)}}. \quad (31)$$

Here, “=0” should be understood as “ $\sim a_0^6$ ” since in general these derivatives are $\sim a_0^5$. These two equations then give us solutions for the leading parameters $c_2^{(1)}$ and $c_2^{(2)}$, once the values of the subleading parameters $c_3^{(s)} \equiv (c_3^{(1)} + c_3^{(2)})/2$ and $\delta c_3 \equiv c_3^{(1)} - c_3^{(2)}$ have been chosen.⁵ However, using Eq. (A5) and the fact that Q_j^2 are independent of $c_3^{(s)}$ [see Eq. (25)], we can show the following dependence of the approximant on $c_3^{(s)}$ (at constant δc_3):

$$d \ln(\sqrt{\mathcal{A}_{\bar{s}}^{[2/2]}}) = d(c_3^{(s)}) \frac{1}{4} (a_1^3 + a_1^2 a_2 + a_1 a_2^2 + a_2^3) + \mathcal{O}(a_j^4) \\ \approx d(c_3^{(s)}) |a_1|^3, \quad (32)$$

where $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3^{(j)}, \dots)$ ($j=1,2$) and we took the index convention $|a_1| \geq |a_2|$. This means that the dependence on $c_3^{(s)}$ cannot be eliminated in the considered case, not even by a PMS variant. In this respect, the situation is analogous to the usual TPS-PMS [2] and the ECH [3] methods. These two methods (see Appendix C), while fixing RScl ($Q_0 \mapsto Q_{\text{ECH}} = Q_{\text{PMS}}$) and c_2 RSch parameter ($c_2^{(0)} \mapsto c_2^{\text{PMS}}$ or c_2^{ECH}) in the original TPS (2), leave the value of the subleading parameter c_3 there unspecified, with the residual c_3 dependence of the (TPS) approximant

$$d \ln(S_{[2]}^{(X)}) \approx d(c_3) a_X^3 / 2, \quad (33)$$

where X stands either for ECH or TPS-PMS. Comparing Eqs. (32) and (33), we see that the $c_3^{(s)}$ dependence of our approximant could be up to twice as strong as that of the TPS-PMS and ECH methods.

Hence, varying $c_3^{(1)}$ and $c_3^{(2)}$ parameters in our approximant at this point would apparently not lead to any new insight. For the sake of simplicity, we choose from now on these two subleading parameters to be equal to each other

$$c_3^{(1)} = c_3^{(2)} \equiv c_3 \quad (\delta c_3 = 0), \quad (34)$$

but we will adjust the common parameter c_3 later to a physically motivated value.

With the chosen restriction (34), the problem of finding our approximant (14) to the TPS (2) basically reduces to the problem of solving the system of three coupled equations (26) and (31) for the three unknowns $y_- [= \beta_0 \ln(Q_1/Q_2)]$

and δc_2 and $c_2^{(s)}$ ($\Leftrightarrow c_2^{(1)}$ and $c_2^{(2)}$). For completeness, the PMS-like equations (31), when $\delta c_3 = 0 = \delta c_4$, are written explicitly in Appendix B, to the relevant order $\sim a_0^5$ at which we solve them—Eqs. (B1),(B2). From there and from Eq. (26) we explicitly see that these three equations contain only the three unknowns (y_- , $c_2^{(s)}$, and δc_2) and the (known) RScl and RSch invariants ρ_2 (24) and $c_1 = \beta_1/\beta_0$. Interestingly enough, these three equations do not depend on c_3 ($= c_3^{(1)} = c_3^{(2)}$). In addition, they do not depend on any other higher order parameters $c_k^{(j)}$ ($k \geq 4$; $j=1,2$) appearing in $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, c_4^{(j)}, \dots)$, except on $\delta c_4 \equiv c_4^{(1)} - c_4^{(2)}$ which was taken to be zero in Eqs. (B1),(B2). Hence, Q_j and $c_2^{(j)}$ ($j=1,2$) will be functions of ρ_2 and c_1 only, thus explicitly RScl and RSch invariant. For simplicity, we want the solutions Q_j^2 and $c_2^{(j)}$ ($j=1,2$) to be independent of *any* higher order parameter $c_k^{(j)}$ ($k \geq 3$) that possibly appears in our approximant, therefore we choose from now on also $\delta c_4 (\equiv c_4^{(1)} - c_4^{(2)}) = 0$. The solution of the mentioned three coupled equations in any specific case can be found numerically, e.g., by using MATHEMATICA or some other comparable software for numerical iteration. Certainly we have to ensure that the program scans through a sufficiently wide range of the initial trial values $y_-^{(\text{in})}$, $(c_2^{(s)})^{(\text{in})}$, and $(\delta c_2)^{(\text{in})}$ for iterations, in order not to miss any solution. The solutions which result in either $|\tilde{\alpha}| \geq 1$ or $|\tilde{\alpha}| \ll 1$ should be discarded since they signal numerical instabilities of the approximant [$|\tilde{\alpha}| \geq 1 \Rightarrow Q_1^2 \approx Q_2^2$ —see Eq. (15)] or are in addition physically unacceptable ($|\tilde{\alpha}| \ll 1 \Rightarrow Q_1^2 \ll Q_2^2$ or $Q_2^2 \ll Q_1^2$). We have apparently two possibilities: (i) y_- , $c_2^{(s)}$, and δc_2 are all real numbers (and thus the initial trial values as well); (ii) $c_2^{(s)}$ and its initial values are real; y_- and δc_2 and their initial values are imaginary numbers ($c_2^{(1)}$ and $c_2^{(2)}$ are complex conjugate to each other, as are Q_1^2 and Q_2^2). In both cases, the approximant itself turns out to be real, as long as c_3 is real.

If we encounter several solutions which give different values for the approximant, we should choose, again within the PMS logic, among them the solution with the smallest curvature with respect to $c_2^{(1)}$ and $c_2^{(2)}$. For such cases, we define two almost equivalent expressions for such curvature in Appendix B—see Eqs. (B4),(B5).

III. BJORKEN POLARIZED SUM RULE (BPSR): c_3 FIXING

We will now apply the described method to the case of the Bjorken polarized sum rule (BPSR) [21]. It is the isotriplet combination of the first moments over x_{Bj} of proton and neutron polarized structure functions

$$\int_0^1 dx_{\text{Bj}} [g_1^{(p)}(x_{\text{Bj}}; Q_{\text{ph}}^2) - g_1^{(n)}(x_{\text{Bj}}; Q_{\text{ph}}^2)] \\ = \frac{1}{6} |g_A| [1 - S(Q_{\text{ph}}^2)], \quad (35)$$

where $p^2 = -Q_{\text{ph}}^2 < 0$ is the momentum transfer carried by the virtual photon. The quantity $S(Q_{\text{ph}}^2)$ has the canonical

⁵Also a value of $\delta c_4 \equiv c_4^{(1)} - c_4^{(2)}$ has to be chosen—see later.

form (1). It has been calculated to the NNLO [22,23], in the $\overline{\text{MS}}$ RSch and with the RScl $Q_0^2 = Q_{\text{ph}}^2$. The pertaining values of r_1 and r_2 , for those Q_{ph}^2 where three quark flavors are assumed active ($n_f = 3$), e.g., at $Q_{\text{ph}}^2 = 3$ or 5 GeV^2 , are $r_1 = 3.5833$ [22] and $r_2 = 20.2153$ [23], so that

$$S_{[2]}(Q_{\text{ph}}^2; Q_0^2 = Q_{\text{ph}}^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}}) = a_0(1 + 3.5833a_0 + 20.2153a_0^2), \quad (36)$$

with

$$a_0 = a(\ln Q_0^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}}, \dots), \quad n_f = 3, \quad c_2^{\overline{\text{MS}}} = 4.471, \\ c_3^{\overline{\text{MS}}} = 20.99. \quad (37)$$

The constant $|g_A|$ appearing in Eq. (35) is known from β -decay measurements [24] (it is denoted there as $|g_A/g_V|$)

$$|g_A| = 1.2670 \pm 0.0035. \quad (38)$$

Solving the coupled system of Eqs. (26) and (B1),(B2) for the three unknowns y_- , $c_2^{(s)}$, and δc_2 , as discussed in the previous section, results in this case in one physical solution only⁶

$$y_- \left(\equiv \frac{1}{2} \beta_0 \ln \frac{Q_1^2}{Q_2^2} \right) = -1.514 \quad (\Rightarrow \tilde{\alpha} = 0.3301), \quad (39) \\ c_2^{(s)} = 3.301, \quad \delta c_2 = -3.672 \Rightarrow c_2^{(1)} = 1.465, \quad c_2^{(2)} = 5.137. \quad (40)$$

Parameter y_+ , defined in Eq. (28), is then obtained from Eq. (27). The resulting scales Q_1 , Q_2 are then 0.767, 1.504 GeV ($Q_{\text{ph}}^2 = 5 \text{ GeV}^2$) and 0.594, 1.165 GeV ($Q_{\text{ph}}^2 = 3 \text{ GeV}^2$). We stress that these results are independent of the value of c_3 (34) and of c_4 and other $c_k^{(j)}$ ($k \geq 5$; $j = 1, 2$) in the approximant $\sqrt{\mathcal{A}_{S^2}}$ (14), and are independent of the choice of RScl Q_0 and RSch ($c_k^{(0)}$, $k \geq 2$) in the original TPS $S_{[2]}$. In TPS (36), the choice was $Q_0 = Q_{\text{ph}}$ and $c_2^{(0)} = c_2^{\overline{\text{MS}}} (= 4.471)$. Knowing Q_j and $c_2^{(j)}$ ($j = 1, 2$), for the actual evaluation of approximant (14) we need to assume a certain value for a_0 (37) (at RScl Q_0). The value of $\tilde{\alpha}$ is obtained from Eq. (16) ($\tilde{\alpha} = 0.3303$); the value of the coupling parameter $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, c_4, c_5^{(j)}, \dots)$ ($j = 1, 2$) can be obtained, for example, by solving the subtracted Stevenson equation (A2)

$$\beta_0 \ln \frac{Q_j^2}{Q_0^2} = \frac{1}{a_j} + c_1 \ln \left(\frac{c_1 a_j}{1 + c_1 a_j} \right) \\ + \int_0^{a_j} dx \frac{(c_2^{(j)} + c_3 x)}{(1 + c_1 x)(1 + c_1 x + c_2^{(j)} x^2 + c_3 x^3)} \\ - \frac{1}{a_0} - c_1 \ln \left(\frac{c_1 a_0}{1 + c_1 a_0} \right) \\ - \int_0^{a_0} dx \frac{(c_2^{\overline{\text{MS}}} + c_3^{\overline{\text{MS}}} x)}{(1 + c_1 x)(1 + c_1 x + c_2^{\overline{\text{MS}}} x^2 + c_3^{\overline{\text{MS}}} x^3)} \\ (j = 1, 2). \quad (41)$$

In Eq. (41) we ignored terms $\propto c_4^{(j)}$ and higher since they are not known ($c_4^{\overline{\text{MS}}}$ is not known, either). Stated otherwise, we set here and in the rest of this section: $c_k^{(1)} = c_k^{(2)} = c_k^{\overline{\text{MS}}} = 0$ for $k \geq 4$, i.e. The β functions pertaining to the approximant are taken in the TPS form to the four-loop order. Hence, the only free parameter in the approximant $\sqrt{\mathcal{A}_{S^2}}$ (14) is now c_3 [cf. condition (34)], all the other nonzero parameters (Q_j^2 , $c_2^{(j)}$, $\tilde{\alpha}$) have been determined and are c_3 - and RScl- and RSch-independent. Further, any effects due to the mass thresholds ($n_f \geq 4$) are ignored in Eq. (41). These effects are suppressed because the difference of the two integrals in Eq. (41) tends to cancel them. Note that the scales appearing in Eq. (41) ($Q_1 \approx 0.6\text{--}0.8 \text{ GeV}$, $Q_2 \approx 1.2\text{--}1.5 \text{ GeV}$, $Q_{\text{ph}} = Q_0 \approx 1.7\text{--}2.2 \text{ GeV}$) are all regarded to be below the threshold ($n_f = 3$) \mapsto ($n_f = 4$), i.e., all the active quark flavors are (almost) massless.⁷

The main question appearing at this point is which value of c_3 ($= c_3^{(1)} = c_3^{(2)}$) should we choose in our approximant? The two most obvious possibilities are $c_3 = 0$ or $c_3 = c_3^{\overline{\text{MS}}}$ ($= 20.99$). The decision is far from being numerically irrelevant. If choosing for $a_0 \equiv a(\ln Q_0^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}})$ at $Q_{\text{ph}}^2 = Q_0^2 = 3 \text{ GeV}^2$ a typical value, e.g., $a_0 = 0.09$ [$\Rightarrow \alpha_s^{\overline{\text{MS}}}(3 \text{ GeV}^2) \approx 0.283$, $\alpha_s^{\overline{\text{MS}}}(M_Z^2) \approx 0.113$], we obtain the following resummed values for the BPSR S

$$\sqrt{\mathcal{A}_{\tilde{S}}^{[2/2]}}(c_3 = 0) = 0.1523, \quad \sqrt{\mathcal{A}_{\tilde{S}}^{[2/2]}}(c_3 = c_3^{\overline{\text{MS}}}) = 0.1632. \quad (42)$$

The latter is 7.16% higher than the former. The corresponding resummed values of the ECH [3] and TPS-PMS [2] are

⁷In the whole paper, we ignore any quark mass effects, except later in the evolution $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2) \mapsto \alpha_s^{\overline{\text{MS}}}(M_Z^2)$ where the quark mass thresholds are significant and accounted for.

⁶Formally, we get two solutions, but they give the same approximant, since the second solution is obtained from the first by $Q_1 \leftrightarrow Q_2$ and $c_2^{(1)} \leftrightarrow c_2^{(2)}$. Further, if ignoring in PMS conditions (B1)–(B2) the denominators, one arrives at two additional solutions, both having $c_2^{(s)} = (6\rho_2 - 7c_1^2/4)/7$; however, one can check that also the denominators are then zero and the derivative (B1) reduces to $2(2\delta c_2 - 15c_1 y_-) \tilde{a}_0^5 / (3y_-)$ which turns out to be finite and nonzero.

$$\mathcal{A}_S^{\text{ECH}}(c_3=0)=0.1535, \quad \mathcal{A}_S^{\text{ECH}}(c_3=c_3^{\overline{\text{MS}}})=0.1593, \quad (43)$$

$$\mathcal{A}_S^{\text{PMS}}(c_3=0)=0.1528, \quad \mathcal{A}_S^{\text{PMS}}(c_3=c_3^{\overline{\text{MS}}})=0.1588. \quad (44)$$

The latter values (for $c_3=c_3^{\overline{\text{MS}}}$) are 3.79% (ECH) and 3.96% (TPS-PMS) higher than the former (for $c_3=0$). Thus, the sensitivity of our approximant to the variation of c_3 is in the considered case almost twice as large as for the ECH and TPS-PMS methods, as anticipated in Eqs. (32),(33) in the previous section. The true value of c_3 in $\mathcal{A}_S^{\text{ECH}}$ should be equal to ρ_3 , i.e., the third RScl and RSch invariant of the BPSR, but this value is not exactly known because the N^3LO coefficient r_3 in the perturbative expansion of the BPSR is not known yet. The stronger c_3 sensitivity should not be regarded as a negative feature of our approximant, but rather within the following context.

Our approximant contains two (RScl invariant) energy scales Q_1, Q_2 . Since the considered observable is close to the nonperturbative sector ($Q_{\text{ph}} < 2.5$ GeV), the relevant scales Q_j ($\sim Q_{\text{ph}}$) are low: $Q_1 \approx 0.6\text{--}0.8$ GeV and $Q_2 \approx 1.2\text{--}1.5$ GeV. Thus the relevant coupling parameters $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3)$ are large: $a_1 \approx 0.19$ and $a_2 \approx 0.11$ (when c_3 is set equal $c_3^{\overline{\text{MS}}}$ and $a_0 = 0.09$, $Q_0^2 = Q_{\text{ph}}^2 = 3$ GeV²). Therefore, the contribution of the c_3 term on the right-hand side of the integrated RGE (41) [\Leftrightarrow differential RGE (3)] at such energy scales is not negligible. This feature, to a somewhat lesser degree, can also be seen in the ECH and TPS-PMS approaches, where $Q_{\text{ECH}} (=Q_{\text{PMS}}) \approx 0.8$ GeV and $a_{\text{ECH}} \equiv a(\ln Q_{\text{ECH}}^2; c_2^{\text{ECH}}, c_3) \approx 0.16$ (when c_3 is set equal to $c_3^{\overline{\text{MS}}}$, and $a_0 = 0.09$, $Q_0^2 = Q_{\text{ph}}^2 = 3$ GeV²). The significant c_3 dependence of all these approximants, at fixed a_0 , reflects the fact that the coupling parameters $a(Q_j)$ appearing in the approximants are not small and that consequently the considered observable is in the low-energy regime. The values of Padé approximants (PA's), when applied to NNLO TPS of an observable (e.g., BPSR), are also c_3 dependent. However, the latter c_3 dependence, in contrast to that in the aforementioned approximants, is not playing a highlighted role, since the PA's depend in addition on the leading RSch parameter c_2 ($\Leftrightarrow c_2^{(0)}$) and even on the RScl Q_0^2 .

The above considerations, however, do not address the important problem presented by Eq. (42): Which value of parameter c_3 should we use in our approximant? We note that c_3 characterizes the N^3LO term in the corresponding β function (3), and the information on its value in a considered approximant cannot be obtained from the NNLO TPS on which the approximant is based. To determine the optimal value of c_3 in an approximant (our, ECH, or TPS-PMS), an important known piece of (nonperturbative) information beyond the NNLO TPS should be incorporated into the approximant. There are at least two natural candidates for this: the location of the leading infrared (IR₁) and ultraviolet (UV₁)

renormalon poles, i.e., the positive and negative poles of the Borel transform $B_S(z)$ of the observable closest to the origin (for a review on renormalons, see Ref. [25]). In the case of the BPSR, these two locations are known from large- β_0 (large- n_f) considerations [26,27]: $z_{\text{pole}} = 1/\beta_0$ (IR₁), $z_{\text{pole}} = -1/\beta_0$ (UV₁).

Which of the two leading renormalons is numerically more important in the BPSR case? In the simple Borel transform of the BjPSR, with $\overline{\text{MS}}$ RSch and RScl $Q_0 = Q_{\text{ph}}$ ($n_f = 3$), the ratio of the residues of the IR₁ and UV₁ poles in the large- β_0 approximation is $2\exp(10/3) \approx 56 \gg 1$ [26,25]. This would suggest strong numerical dominance of the IR₁ over UV₁. However, when using there the V scheme [1], i.e., $\overline{\text{MS}}$ with RScl $Q_0 = Q_{\text{ph}} \exp(-5/6)$ ($\approx Q_{\text{ECH}}$), this ratio goes down to 2. This would suggest that the UV₁ (*vis à vis* IR₁) is not entirely negligible. The authors of Ref. [27] used the 't Hooft RSch and varied the RScl in such an approach (large- β_0 , simple Borel transform, principal value prescription), and their Fig. 2 for the BjPSR at $Q_{\text{ph}}^2 = 2.5$ GeV² suggests that IR renormalon contributions to $S(Q_{\text{ph}}^2)$ are 3–4 times larger than those of the UV renormalons. The relative strength of the UV vs IR renormalon contributions, in the RScl or RSch noninvariant approach with simple Borel transform, appears to depend in practice on the choice of the RScl and RSch. Incidentally, a consideration of the status of the renormalon contributions and of their scheme dependence was made in Ref. [28]. The question of the relative suppression of the (leading) UV renormalon contributions in RScl- and RSch-invariant resummations would deserve a further study. An additional uncertainty resides in the fact that the residues, in contrast to the renormalon pole locations, change and thus attain unknown values when we go beyond the large- β_0 approximation. For the UV renormalons, this uncertainty shows up in an especially acute form [29].

The aforementioned works, however, suggest strongly that, in the BPSR case $S(Q_{\text{ph}}^2 = 3\text{--}5$ GeV²), we should preferably fix the value of c_3 in our, ECH, and TPS-PMS resummation approximants by using IR₁ ($z_{\text{pole}} = 1/\beta_0$) and not UV₁ ($z_{\text{pole}} = -1/\beta_0$) information. The IR₁ pole location can be transcribed as $y_{\text{pole}} = 2$, where $y \equiv 2\beta_0 z$. This corresponds to possible renormalon-ambiguity contributions $\sim 1/Q_{\text{ph}}^2$ to the BPSR observable which are nonperturbative.

We will present now an algorithm for adjusting approximately the value of c_3 in our approximant for the NNLO TPS (2). Briefly, it consists of the requirement that c_3 must be adjusted in such a way that the Borel transform of the approximant has the correct known location of the lowest positive pole, where the latter location is obtained by construction of Padé approximants (PA's) of the Borel transform.

A first idea would be to use simple Borel transforms. We would first expand our approximant (with a general yet unspecified c_3) in power series of a coupling parameter, say $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots)$, up to a certain order $\sim a_0^{j+1}$ ($j \geq 3$), then obtain from this predicted $S_{[j]}$ TPS the corresponding $\mathcal{B}_{[j]}(z)$ TPS (up to $\sim z^j$) of the simple Borel transform as schematically described by

$$\begin{aligned}
\sqrt{\mathcal{A}_S^{[2/2]}}(a_0; c_3) &= S_{[j]}^{\text{pr}}(a_0; c_3) \\
&= a_0 [1 + r_1 a_0 + r_2 a_0^2 + r_3^{\text{pr}}(c_3) a_0^3 + \dots \\
&\quad + r_j^{\text{pr}}(c_3) a_0^j], \quad (45) \\
&\Rightarrow \mathcal{B}_{[j]}^{\text{pr}}(z; c_3) \\
&= 1 + \frac{r_1}{1!} z + \frac{r_2}{2!} z^2 + \frac{r_3^{\text{pr}}(c_3)}{3!} z^3 \\
&\quad + \dots + \frac{r_j^{\text{pr}}(c_3)}{j!} z^j. \quad (46)
\end{aligned}$$

The (approximate) pole structure of the simple Borel transform can be investigated by constructing various PA's of its TPS (46). The requirement that the lowest positive pole be at $y(\equiv 2\beta_0 z) = 2.0$ would then give us predictions for c_3 . However, this approach is in practice seriously hampered, because coefficients $r_k/k!$ of the simple Borel transform $\mathcal{B}(z; c_3)$ depend very much on the choice of the RScl (Q_0^2) and RSch ($c_2^{(0)}, c_3^{(0)}, \dots$). For example, if expanding our approximant $\sqrt{\mathcal{A}_S^{[2/2]}}(a_0; c_3)$ up to $\sim a_0^4$ in an RSch with $c_2^{(0)} = c_2^{\text{MS}}$ and an arbitrary $c_3^{(0)}$, and keeping the RScl Q_0^2 unchanged ($= Q_{\text{ph}}^2$), we reproduce in the BPSR case the first two coefficients r_1 and r_2 of Eq. (36), while the predicted r_3 in this RSch is

$$r_3^{\text{pr}} = 125.790 \dots - \frac{c_3^{(0)}}{2} + c_3. \quad (47)$$

The PA's [2/1] or [1/2] of the corresponding simple Borel transform TPS $\mathcal{B}_{[3]}^{\text{pr}}(z)$ would therefore be functions of $(-c_3^{(0)}/2 + c_3)$, and the requirement $y_{\text{pole}} = 2.0$ would at this level give us only a prediction for $(-c_3^{(0)}/2 + c_3)$, not for c_3 itself.⁸ For example, working with $\mathcal{B}_{[3]}^{\text{pr}}(z)$ in the RSch with $c_3^{(0)} = 0$ results in a prediction for c_3 that is by about 10.5 lower than the one when $c_3^{(0)} = c_3^{\text{MS}} (\approx 21)$ is used. If using the ECH $a_{\text{ECH}}(c_3)$ [3] or TPS-PMS $S_{\text{PMS}}(c_3)$ [2] approximants instead of our approximant (where c_3 is the arbitrary subleading parameter used in a_{ECH} and a_{PMS} —see Appendix C), the corresponding prediction with $Q_0 = Q_{\text{ph}}$ is $r_3^{(\text{pr})} = 129.8998 \dots + (-c_3^{(0)} + c_3)/2$. Hence, also in the case of these approximants we end up with the same kind of problem of strong RSch dependence ($c_3^{(0)}$ dependence) of the predicted values of c_3 .

Therefore, we will use a variant of the RScl- and RSch-independent Borel transform $B(z)$ introduced by Grunberg [30], who in turn introduced it on the basis of the modified Borel transform of the authors of Ref. [31]

⁸The [1/1] PA of the simple Borel transform is independent of c_3 and of $c_3^{(0)}$. In the BPSR case, in the modified minimal subtraction (MS) RSch and at RScl $Q_0^2 = 3$ or 5 GeV², where $n_f = 3$, it predicts $y_{\text{pole}} \approx 1.6$.

$$S(Q_{\text{ph}}^2) = \int_0^\infty dz \exp[-\rho_1(Q_{\text{ph}}^2)z] B_S(z). \quad (48)$$

Here, ρ_1 is the first Stevenson's RScl or RSch invariant (23) of the observable S :

$$\rho_1(Q_{\text{ph}}^2) = -r_1(Q_{\text{ph}}^2/Q_0^2) + \beta_0 \ln \frac{Q_0^2}{\bar{\Lambda}^2} = \beta_0 \ln \frac{Q_{\text{ph}}^2}{\bar{\Lambda}^2}, \quad (49)$$

where $\bar{\Lambda}$ is the universal scale appearing in the Stevenson equation (A1), while $\bar{\Lambda}$ is a scale which depends on the choice of the observable S . But $\bar{\Lambda}$ is independent of RScl Q_0 and of RSch and even of the process momentum Q_{ph} . We note that $\rho_1(Q_{\text{ph}}^2)$ is, up to a constant c (the latter is irrelevant for the position of the poles of B_S), equal to $1/a^{(1\text{-loop})}(Q_{\text{ph}}^2)$. Thus, $B_S(z)$ of Eq. (48) reduces to the simple Borel transform, up to a factor $\exp(cz)$, if higher than one-loop effects are ignored. The positions of the poles of $B_S(z)$ of Eq. (48) are the same as those of the simple Borel transform. The coefficients of the power expansion of $B_S(z)$ of Eq. (48) are RScl and RSch invariant, in contrast to the case of the simple Borel transform. These invariant coefficients can be related with coefficients r_n of S with relative ease in a specific RSch $c_k = c_1^k$ ($k = 2, 3, 4, \dots$), while keeping the RScl Q_0^2 unchanged

$$\begin{aligned}
B_S(z) &= (c_1 z)^{c_1 z} \exp(-r_1 z) \sum_0^\infty \frac{(\tilde{r}_n - c_1 \tilde{r}_{n-1})}{\Gamma(n+1+c_1 z)} z^n \\
&\equiv (c_1 z)^{c_1 z} \bar{B}_S(z). \quad (50)
\end{aligned}$$

Here, \tilde{r}_n is the coefficient at \tilde{a}^{n+1} in the expansion of S in powers of $\tilde{a} \equiv a(\ln Q_0^2; c_1^2, c_1^3, c_1^4, \dots)$, and by definition $\tilde{r}_{-1} = 0$, $\tilde{r}_0 = 1$. In Eq. (50), we introduced the modified RScl or RSch invariant Borel transform $\bar{B}_S(z)$, by extracting the factor $(c_1 z)^{c_1 z}$ whose behavior at $z \rightarrow 0$ may be problematic for PA's to deal with.⁹ The obtained coefficients of the power expansion of $\bar{B}_S(z)$ are explicitly RScl and RSch invariant, depending only on the invariants ρ_j ($j \geq 2$), on c_1 and on some universal constants.

We will now calculate the invariant Borel transform $\bar{B}_{\sqrt{\mathcal{A}}}$ of our approximant. The coefficients \tilde{r}_k as predicted by our approximant (14) $\sqrt{\mathcal{A}_S^{[2/2]}}(c_3)$ are functions of the only un-

⁹Grunberg's [30] Borel transform $\bar{B}^{(\text{Gr})}$ was chosen by convention as $\bar{B}^{(\text{Gr})}(z) = \Gamma(1+c_1 z) \exp(c_1 z) \bar{B}(z)$. In this way, $\bar{B}^{(\text{Gr})}(z) \approx B(z) \sqrt{2\pi c_1 z}$ when $z \rightarrow \infty$, and the coefficients of the power expansion of $\bar{B}^{(\text{Gr})}$ in z depend only on the RScl/RSch invariants ρ_j (no dependence on c_1 and on Γ -function-related constants). We decided not to follow this convention, primarily since $\Gamma(1+c_1 z)$ introduces spurious poles on the negative axis, the one closest to the origin being $y(\equiv 2\beta_0 z) \approx -2.53$. Such spurious poles not far away from the origin can significantly limit the PA's ability to locate correctly the leading IR renormalon pole ($y_{\text{pole}} \approx 2.0$).

TABLE I. Predictions for c_3 in our, ECH, and TPS-PMS approximants, using various PA's of the invariant Borel transform $\bar{B}(z)$ of the approximants and demanding that the lowest positive pole be at $z_{\text{pole}}=1/\beta_0$ ($=4/9$). The higher order parameters $c_k^{(j)}$ ($k \geq 4$, $j=1,2$) in our approximant, and c_k ($k \geq 4$) in ECH and TPS-PMS, were all set equal to zero.

PA $_{\bar{B}}$	$c_3(\sqrt{\mathcal{A}_{S^2}})$	c_3 (ECH)	c_3 (TPS-PMS)
[2/1]	21.7	35.1	35.1
[3/1]	13.7	19.5	19.0
[4/1]	11.1	14.4	13.1
[5/1]	9.3	11.2	8.8
[1/2]	12.8	17.3	17.3
[2/2]	12.4	16.9	16.2
[3/2]	$11.7 \pm 3.4i$	$15.8 \pm 6.4i$	$15.4 \pm 7.4i$
[4/2]	$10.3 \pm 2.8i$	$12.9 \pm 5.1i$	$11.6 \pm 6.8i$
[1/3]	12.4	16.9	16.2
[2/3]	12.9	17.4	$18.3 \pm 0.8i$
[3/3]	$10.6 \pm 2.9i$	$13.6 \pm 5.5i$	$12.6 \pm 7.0i$
average	≈ 12.5	≈ 17.0	≈ 16.0

known c_3 [$\tilde{r}_k = \tilde{r}_k(c_3)$, $k \geq 3$], They can be obtained as coefficients of the power expansion of $\sqrt{\mathcal{A}_{S^2}}(c_3)$ in powers of \tilde{a} . Looking back at the form (14) of our approximant, such a power expansion requires first the separate expansions of $a_1 = a(Q_1^2; c_2^{(1)}, c_3, 0, \dots)$ and of $a_2 = a(Q_2^2; c_2^{(2)}, c_3, 0, \dots)$ in powers of \tilde{a} . The latter expansions can be read off Eq. (A7), up to $\sim \tilde{a}^5$ (there $a \rightarrow a_1$ or a_2 and $a_0 \rightarrow \tilde{a}$). In fact, we carried out the latter expansion up to $\sim \tilde{a}^8$ (with the help of MATHEMATICA), which allowed us to write the approximant $\sqrt{\mathcal{A}_{S^2}}(c_3)$ up to $\sim \tilde{a}^7$. This in turn leads us to obtain the invariant Borel transform $B_{\sqrt{\mathcal{A}}}(z)$ up to $\sim z^6$, according to Eq. (50), and allows us to construct PA's of the Borel transform of as high order as [3/3], [2/4], [5/1]. The coefficients starting at z^3 are predictions of the approximant and are c_3 dependent: $\bar{B}_3(z) = 1 + \bar{b}_1 z + \bar{b}_2 z^2 + \bar{b}_3(c_3) z^3 + \dots$, with $\bar{b}_1 \approx -0.7516$, $\bar{b}_2 \approx 0.4209$, $\bar{b}_3(c_3) \approx (-2.664 + 0.1667c_3)$, etc. Construction of various PA's of that Borel transform and requirement that the smallest positive pole equal $y_{\text{pole}} (=2\beta_0 z_{\text{pole}}) = 2.0$ gives us predictions for c_3 which are listed for the described case in the second column of Table I. In the column we included values of c_3 with small nonzero imaginary parts and $\text{Re}(c_3) \approx 10-12$, since for such values the PA $_{\bar{B}}$'s and the TPS of \bar{B} are almost real, with imaginary parts less than 1% of the real part for $y < 1.9$. In the latter cases the real part of c_3 may be regarded as the suggested value. The actual value of c_3 must be exactly real, but since a specific PA predicts only an approximate value of c_3 , this latter value is not necessarily exactly real. We did not include some other solutions which differ a lot from those given in the column. Predictions of PA $_{\bar{B}}$'s of the intermediate orders ([3/1], [4/1], [2/2], [3/2], [1/3], [2/3]) give us the average value $c_3 \approx 12.5$ which we will adopt. The prediction by PA [2/1] differs from most of the other predictions, apparently because [2/1] is of low order. Predictions by the high-

est PA's ([5/1], [4/2], [3/3]) also differ from the average. The reason for this probably lies in the fact that these PA's contain information on many higher order coefficients \tilde{r}_n ($n=3,4,5,6$) which are not contained in the TPS $S_{[2]}$ on which the approximant $\sqrt{\mathcal{A}_{S^2}}$ is based. In addition, these high order PA's are implicitly dependent on the high order parameters $c_k^{(1)}$ and $c_k^{(2)}$ ($k=4,5,6,7$) which were here simply set equal to zero (we will come back to this point later in Sec. V).

Completely analogous considerations produce the values of c_3 parameter in the ECH and TPS-PMS approximants. For details on the ECH and TPS-PMS methods, when applied to the NNLO TPS $S_{[2]}$ (2), we refer to Appendix C. Also in this case, we make for the corresponding β functions the simple TPS choice ECH RSch= $(\rho_2, c_3, 0, \dots)$; TPS-PMS RSch= $(3\rho_2/2, c_3, 0, \dots)$. The obtained predictions for c_3 for these approximants are included in Table I. Again, PA [2/1] and the highest order PA's appear to give unreliable predictions. On the basis of the predictions of PA $_{\bar{B}}$'s of intermediate order, we will adopt the value $c_3 = 17$ for the ECH case, and $c_3 = 16$ for the TPS-PMS case. The actual values of c_3 must be exactly real.

In fact, we can apply this method of determining the c_3 parameter of our approximant (and of ECH and TPS-PMS approximants) to any QCD observable given at the NNLO and whose leading IR renormalon pole is known via large- β_0 considerations. The method, however, is well motivated only if there are indications that the leading IR renormalon contributions to the observable are larger than those of the leading UV renormalon. We wish to stress that our approximant, as well as the ECH and TPS-PMS approximants, are completely independent of the original choice of the RScl and RSch in the TPS of the observable, because the parameter c_3 is RScl and RSch invariant since it is determined by using the RScl- and RSch-invariant Borel transform $\bar{B}(z)$.

A few remarks about the multiplicity of the discussed IR $_1$ pole are in order. The simple Borel transform $\Sigma r_k z^k / k!$ of $S(Q_{\text{ph}}^2)$ behaves near $z_{\text{pole}} (=1/\beta_0)$ as $\sim 1/(z_{\text{pole}} - z)^\kappa$ where the multiplicity is [32,34,29] $\kappa = 1 + (\beta_1/\beta_0)z_{\text{pole}} + (\gamma/\beta_0)$, and γ is the one-loop anomalous dimension of the corresponding two-dimensional operator appearing in the operator product expansion for S (usually $\gamma \geq 0$). On the other hand, the RScl- and RSch-invariant Borel transform (50) behaves near z_{pole} with the simpler pole multiplicity [31] $\kappa = 1 + (\gamma/\beta_0)$. To our knowledge, the anomalous dimension γ is not known in this case. However, in the case of the Adler function (logarithmic derivative of the correlation function of quark current operators), the one-loop anomalous dimension of the four-dimensional operator corresponding to the lowest IR renormalon pole there ($z_{\text{pole}} = 2/\beta_0$) is known [32,33] to be $\gamma = 0$. If $\gamma = 0$ also in the BPSR case, then the RScl- and RSch-invariant Borel transform (48)–(50) has $\kappa = 1$, i.e., the leading IR renormalon pole is a simple pole, in contrast to the simple Borel transform where κ is noninteger. In such a case, we may have an additional incentive to use, instead of the simple Borel transform, the invariant Borel transform (48)–(50) in conjunction with the aforescribed PA's of Table I. Namely, PA's are very good at discerning the loca-

tion of a pole if such a pole is simple, and are somewhat less successful in this job if the pole is multiple or with noninteger multiplicity.

IV. BPSR: PREDICTIONS FOR THE COUPLING PARAMETER

Now that we have fixed the values of the c_3 parameter in the approximants $\sqrt{\mathcal{A}_{S^2}(a_0; c_3)}$, ECH and TPS-PMS, the only adjustable parameter in them is the numerical value of $a_0 \equiv \alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)/\pi$, at such Q_{ph}^2 where three flavors are assumed active, e.g., at $Q_{\text{ph}}^2 = 3$ or 5 GeV^2 . This a_0 can be obtained by requiring that it should reproduce the experimental values for $S(Q_{\text{ph}}^2)$ of Eq. (35). The questions connected with the extraction of the values of the BPSR integral (35) from the measured polarized structure functions are at present not quite settled. One source of the uncertainty arises from the fact that these structure functions have not been measured at small values of x_{Bj} and that, therefore, a theoretical extrapolation to such small x_{Bj} values is needed. The authors of Refs. [35,36] used the small- x_{Bj} extrapolation as suggested by the Regge theory, the assumption made also by various experimentalist groups before 1997. The values thus obtained in Refs. [35,36], on the basis of measurements at SLAC and CERN before 1997, are

$$\text{(Regge): } \frac{1}{6} |g_A| [1 - S(Q_{\text{ph}}^2 = 3 \text{ GeV}^2)] = 0.164 \pm 0.011. \quad (51)$$

On the other hand, the authors of Ref. [37] used a small- x_{Bj} extrapolation based on the NLO version of the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equations [perturbative QCD (PQCD)] as opposed to the Regge extrapolation (see also Ref. [38]). This leads to higher values and larger uncertainties of the BPSR integral. The values extracted in this way by [37] (their Table 4), based on SLAC data, are

$$\text{(II): } \frac{1}{6} |g_A| [1 - S(Q_{\text{ph}}^2 = 3 \text{ GeV}^2)] = 0.177 \pm 0.018. \quad (52)$$

Furthermore, most of the experimentalist groups have adopted, since 1997, similar NLO PQCD approaches to the small- x_{Bj} extrapolation, e.g., SMC Collaboration [39] at CERN, E154 [40] and E155 [19] Collaborations at SLAC. The most recent and updated measurements of the polarized structure functions are those of Ref. [19]. Their combined value of the BPSR integral at $Q_{\text{ph}}^2 = 5 \text{ GeV}^2$ is

$$\text{(I): } \frac{1}{6} |g_A| [1 - S(Q_{\text{ph}}^2 = 5 \text{ GeV}^2)] = 0.176 \pm 0.008. \quad (53)$$

Apart from the problem of the small- x_{Bj} extrapolation, there is a problem of accounting for nuclear effects. Since the extraction of the $g_1^{(n)}$ structure function is based on the measurements of the structure functions of the deuteron and ^3He , nuclear effects have to be taken into consideration. The (multiplicative) effects due to the nuclear wave function

have been taken into account in Eqs. (53) and (52). However, recently the authors of Ref. [41] argued that additional nuclear effects, originating from spin-one isosinglet 6-quark clusters in deuteron and helium (which include the shadowing, EMC, and Fermi motion effects), affect the extracted values of the neutron structure function $g_1^{(n)}$ in such a way that the value of the BPSR integral increases by about 10%. This would then change the E155 values of Eq. (53) to

$$\text{(I'): } \frac{1}{6} |g_A| [1 - S(Q_{\text{ph}}^2 = 5 \text{ GeV}^2)] = 0.193 \pm 0.009. \quad (54)$$

The values of Eq. (52), at $Q_{\text{ph}}^2 = 3 \text{ GeV}^2$ would be increased to about 0.195 ± 0.020 . We will not consider this case II' and case I' (54) for the time being, but will briefly return to them in Sec. VI.

In the following we will extract the values of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ from the BPSR-integral values (53) and (52), and will simply denote the corresponding cases as I and II, respectively.

If we insert the value (38) for $|g_A|$ into Eqs. (53) and (52), we obtain

$$\text{(I): } S(Q_{\text{ph}}^2 = 5 \text{ GeV}^2) = 0.167 \pm 0.038, \quad (55)$$

$$\text{(II): } S(Q_{\text{ph}}^2 = 3 \text{ GeV}^2) = 0.162 \pm 0.085. \quad (56)$$

The present small uncertainty in the value of $|g_A|$ (38) practically does not contribute to the uncertainties of $S(Q_{\text{ph}}^2)$ in Eqs. (55),(56).

Our approximant gives, for example, for $a_0 \equiv a(\ln 3 \text{ GeV}^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}}, 0, \dots) = 0.09 [\Leftrightarrow \alpha_s^{\overline{\text{MS}}}(Q^2 = 3 \text{ GeV}^2) \approx 0.283]$ the value 0.1585, which is not far from the middle values in Eqs. (55),(56). Varying a_0 in our approximant (with $c_3 = 12.5$) in such a way that the middle and the endpoint values of the right-hand side of Eqs. (55) or (56) are reproduced then results in the following predictions for α_s (in $\overline{\text{MS}}$ RSch):

$$\alpha_s^{\overline{\text{MS}}}(Q^2 = 5 \text{ GeV}^2) = 0.2894_{-0.0345}^{+0.0238} \quad \text{(I);}$$

$$\alpha_s^{\overline{\text{MS}}}(Q^2 = 3 \text{ GeV}^2) = 0.2855_{-0.1024}^{+0.0450} \quad \text{(II).} \quad (57)$$

We then evolved these predicted values via four-loop RGE (3) to $Q^2 = M_Z^2$, using the values of the four-loop coefficient $c_3(n_f)$ in the $\overline{\text{MS}}$ RSch [42] and the corresponding three-loop matching conditions [43] for the flavor thresholds. We used the matching at $\mu(n_f) = \kappa m_q(n_f)$ with the choice $\kappa = 2$, where $m_q(n_f)$ is the running quark mass $m_q(m_q)$ of the n_f th flavor and $\mu(n_f)$ is defined as the scale above which n_f flavors are active.¹⁰ The resulting predictions for $\alpha_s(M_Z^2)$ are

¹⁰If increasing κ from 1.8 to 3 in case I, the predictions for the central, upper, lower values of $\alpha_s(M_Z^2)$ decrease by 0.12, 0.15, 0.09 %, respectively; increasing κ from 1.5 to 3 in case II, the respective numbers are 0.12, 0.17, 0.03 %. We assumed $m_c(m_c) = 1.25 \text{ GeV}$ and $m_b(m_b) = 4.25 \text{ GeV}$.

TABLE II. Predictions for $\alpha_s^{\overline{\text{MS}}}$, derived from various resummation approximants to the BPSR at $Q_{\text{photon}}^2 = 5 \text{ GeV}^2$, 3 GeV^2 . Predictions for the case I (53) and II (52) are given in parallel.

Approximant	$\alpha_s(5 \text{ GeV}^2)$: (I)	$\alpha_s(3 \text{ GeV}^2)$: (II)	$\alpha_s(M_Z^2)$: (I)	$\alpha_s(M_Z^2)$: (II)
NNLO TPS	$0.3287^{+0.0465}_{-0.0530}$	$0.3221^{+0.0989}_{-0.1341}$	$0.1252^{+0.0055}_{-0.0078}$	$0.1183^{+0.0095}_{-0.0232}$
N ³ LO TPS ($r_3 = 128.05$)	$0.3121^{+0.0393}_{-0.0464}$	$0.3065^{+0.0823}_{-0.1215}$	$0.1230^{+0.0050}_{-0.0073}$	$0.1163^{+0.0089}_{-0.0219}$
[1/2] _S (NNLO)	$0.3054^{+0.0339}_{-0.0426}$	$0.3003^{+0.0693}_{-0.1155}$	$0.1220^{+0.0046}_{-0.0069}$	$0.1155^{+0.0079}_{-0.0212}$
[2/1] _S (NNLO)	$0.3006^{+0.0316}_{-0.0404}$	$0.2959^{+0.0637}_{-0.1118}$	$0.1213^{+0.0044}_{-0.0066}$	$0.1149^{+0.0075}_{-0.0208}$
$\sqrt{[2/2]_{S^2}}$ (NNLO)	$0.2937^{+0.0271}_{-0.0369}$	$0.2895^{+0.0533}_{-0.1061}$	$0.1203^{+0.0039}_{-0.0063}$	$0.1140^{+0.0066}_{-0.0200}$
[2/2] _S (N ³ LO, $r_3 = 128.05$)	$0.2944^{+0.0282}_{-0.0375}$	$0.2901^{+0.0561}_{-0.1067}$	$0.1204^{+0.0040}_{-0.0063}$	$0.1141^{+0.0069}_{-0.0201}$
TPS-PMS (NNLO, $c_3 = 16.0$)	$0.2907^{+0.0259}_{-0.0354}$	$0.2867^{+?}_{-0.1035}$	$0.1198^{+0.0038}_{-0.0060}$	$0.1136^{+?}_{-0.0197}$
ECH (NNLO, $c_3 = 17.0$)	$0.2898^{+0.0244}_{-0.0348}$	$0.2859^{+0.0468}_{-0.1028}$	$0.1196^{+0.0037}_{-0.0059}$	$0.1135^{+0.0060}_{-0.0196}$
$\sqrt{\mathcal{A}_{S^2}^{[2/2]}}$ (NNLO, $c_3 = 12.5$)	$0.2894^{+0.0238}_{-0.0345}$	$0.2855^{+0.0450}_{-0.1024}$	$0.1196^{+0.0035}_{-0.0059}$	$0.1135^{+0.0058}_{-0.0196}$
TPS-PMS (NNLO, $c_3 = 0.0$)	$0.2957^{+0.0296}_{-0.0380}$	$0.2913^{+?}_{-0.1077}$	$0.1206^{+0.0042}_{-0.0064}$	$0.1143^{+?}_{-0.0203}$
ECH (NNLO, $c_3 = 0.0$)	$0.2947^{+0.0273}_{-0.0373}$	$0.2904^{+0.0537}_{-0.1068}$	$0.1204^{+0.0039}_{-0.0062}$	$0.1142^{+0.0066}_{-0.0202}$
$\sqrt{\mathcal{A}_{S^2}^{[2/2]}}$ (NNLO, $c_3 = 0.0$)	$0.2960^{+0.0278}_{-0.0378}$	$0.2916^{+0.0545}_{-0.1078}$	$0.1206^{+0.0040}_{-0.0063}$	$0.1143^{+0.0067}_{-0.0202}$

$$\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.1196^{+0.0035}_{-0.0059} \quad (\text{I}); \quad 0.1135^{+0.0058}_{-0.0196} \quad (\text{II}). \quad (58)$$

In Table II, we give the values of $\alpha_s^{\overline{\text{MS}}}$ as predicted from the BPSR data (55) and (56) by our approximant (with $c_3 = 12.5$), by the ECH (with $c_3 = 17$), and by the TPS-PMS (with $c_3 = 16$). For comparison, we include predictions of these three approximants when c_3 in them is set equal to zero, i.e., for the case when the location of the leading IR renormalon (IR₁) pole in these approximants is not correct. Given are always three predictions for α_s , corresponding to the three values of S (55) for case I, and (56) for case II. In addition, predictions of the following approximants are included in Table II: TPS $S_{[2]}$ (36) (NNLO TPS); TPS $S_{[3]}$ with $r_3 = 128.05$ (N³LO TPS); off-diagonal Padé approximants (PA's) [1/2]_S and [2/1]_S, both based solely on the NNLO TPS $S_{[2]}$ (36); square root of the diagonal PA (DPA) [2/2]_{S²}, which is based solely on the NNLO TPS (36); [2/2]_S is the DPA constructed on the basis of the N³LO TPS $S_{[3]}$ with $r_3 = 128.05$. For [2/2]_S and N³LO TPS we chose the latter value of r_3 (in $\overline{\text{MS}}$, at RScl $Q_0^2 = Q_{\text{ph}}^2$, $n_f = 3$) because then the [1/2] PA of the invariant Borel transform \overline{B}_S (50) predicts the IR₁ pole $y_{\text{pole}} = 2.0$. We wrote in Table II numbers with four digits in order to facilitate a clearer comparison of predictions of various methods.

From Table II we see that the values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ predicted by various approximants differ significantly from each other. Addition of the N³LO term in the TPS decreases the central value of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ by 0.0022 (0.0020 in case II), and application of the NNLO dPA approximant [2/2]_{S²} decreases this value by a further 0.0027 (0.0023). Our approximant $\sqrt{\mathcal{A}_{S^2}}(c_3 = 12.5)$, which is an RScl- and RSch-invariant extension of the method of the DPA [2/2]_{S²}, decreases the central $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ by a further amount of 0.0007 (0.0005). Predictions of the ECH and TPS-PMS methods are very close to those of our method if the value of c_3 in them is adjusted in the aforesaid way. However, predictions of these two and of our method increase and

come closer to the predictions of the NNLO DPA once we simply set in these approximants $c_3 = 0$, thus abandoning the requirement of the correct location of the IR₁ pole. The predictions of the N³LO DPA [2/2]_S are almost identical with those of the NNLO DPA. All the PA resummations were carried out with the RScl $Q_0^2 = Q_{\text{ph}}^2$ ($n_f = 3$) and in $\overline{\text{MS}}$ RSch, and their predictions would change somewhat if the RScl and RSch were changed—in contrast to the presented predictions of $\sqrt{\mathcal{A}_{S^2}}$, ECH and TPS-PMS.

We wish to point out that the $\alpha_s^{\overline{\text{MS}}}$ predictions for the case II (52) were already presented in the short version [18]. However, they were somewhat lower there [the central values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ were lower by about 0.0009–0.0011]—because the value of the β -decay parameter $|g_A|$ there was taken from the Particle Data Book of 1994 $|g_A| = 1.257(\pm 0.2\%)$ (used also in [37]), while the value used here (38) is the updated value based on Ref. [24].

In Fig. 1(a) we present various approximants for $S(Q_{\text{ph}}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ ($n_f = 3$, e.g., $Q_{\text{ph}}^2 = 3$ or 5 GeV^2), and in Fig. 1(b) the approximants for $S(5 \text{ GeV}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$. There is one peculiarity of the (NNLO) TPS-PMS method, as seen also in Figs. 1—for high values of observable S this method does not give solutions. This is so because the polynomial form of the (NNLO) TPS-PMS S^{PMS} [see Eq. (C4)] is bounded from above by $S_{\text{max}}^{\text{PMS}} = (2/3)^{3/2} \rho_2^{-1/2}$ which, in the considered case ($\rho_2 = 5.476$), is equal to 0.233 which is below $S_{\text{max}} = 0.247$ in case II (see Appendix C for more details). This is also indicated in Table II.

We wish to emphasize one aspect that makes the approximant $\sqrt{\mathcal{A}_{S^2}}$ conceptually quite different from the DPA [2/2]_S. Although both approximants incorporate information about the location of the IR₁ pole ($y_{\text{pole}} = 2$), they do it in two very different ways. The DPA [2/2]_S is constructed on the basis of the N³LO TPS with $r_3 = 128.05$, where only this latter coefficient contains approximate information on the pole's location. So this DPA is a pure N³LO construction and is RSch and even RScl dependent (weakly). The approx-

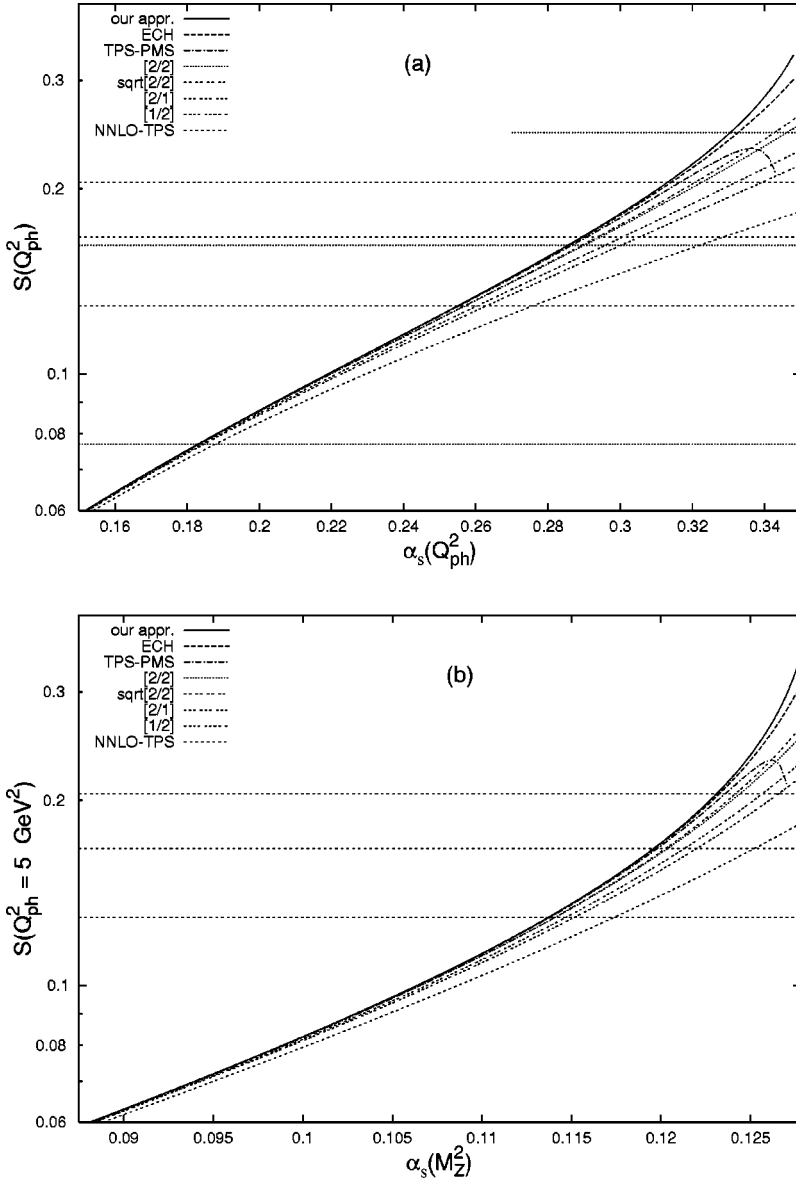


FIG. 1. Predictions of various approximants: (a) for $S(Q_{\text{ph}}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ when $n_f=3$; (b) for $S(Q_{\text{ph}}^2=5 \text{ GeV}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$. The values of the c_3 parameter in our approximant ($c_3=12.5$), ECH ($c_3=17.0$), and TPS-PMS ($c_3=16.0$) have been adjusted to ensure the correct location of the leading IR renormalon pole. The experimental bounds S_{min} , S_{max} , and S_{mid} are indicated as dashed horizontal lines for case I (55) ($Q_{\text{ph}}^2=5 \text{ GeV}^2$) and dotted horizontal lines for case II (56) ($Q_{\text{ph}}^2=3 \text{ GeV}^2$).

imant $\sqrt{\mathcal{A}_{S^2}}$ is constructed on the basis of the NNLO TPS. It is a RScl and $c_2^{(0)}$ independent NNLO construction, and the correct IR₁ pole location is obtained by the adjustment of the c_3 parameter within the approximant. As argued previously [see the second paragraph after Eq. (44)], the c_3 dependence in $\sqrt{\mathcal{A}_{S^2}}(c_3)$ is closely related with the sensitivity of the approximant to the details of the RGE evolution, and the latter details are the more important the more nonperturbative the observable is. So it seems very natural that it is the intrinsic c_3 parameter in $\sqrt{\mathcal{A}_{S^2}}(c_3)$ that parametrizes the (nonperturbative) IR₁ pole location, and at the same time it makes the approximant fully RSch independent. The same is true for the ECH and the TPS-PMS approximants.

On the other hand, it would be an ambiguous approach to implement this kind of c_3 fixing in the NNLO PA methods ($[1/2]_S$, $[2/1]_S$, $[2/2]_{S^2}^{1/2}$)—because these resummations depend in addition on the leading RSch parameter c_2 ($\Leftrightarrow c_2^{(0)}$) and even on the RScl Q_0^2 . Therefore, it may not be so surprising that the results of our method, ECH, and TPS-PMS,

with the mentioned c_3 fixing, all give predictions that are clustered closely together and are significantly distanced from the predictions of (D)PA's.

There is another theoretical aspect which indicates that the predictions of the (NNLO) approximant $\sqrt{\mathcal{A}_{S^2}}$ should in general be better than those of the (NNLO) DPA $[2/2]_{S^2}^{1/2}$. Namely, the latter DPA is just a one-loop approximation to our approximant. More specifically, DPA $[2/2]_{S^2}^{1/2}$ is similar to ansatz (14), but each $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, \dots)$ is replaced by the coupling parameter $a^{(1-1)}(\ln \bar{Q}_j^2)$ evolved from the RScl Q_0^2 to a \bar{Q}_j^2 by the one-loop RGE in the original ($\overline{\text{MS}}$) RSch. This follows from considerations in Refs. [15,16], and can also be checked directly as indicated in the paragraph after Eqs. (9)–(11). The DPA $[2/2]_{S^2}^{1/2}$ possesses residual RScl dependence, and RSch dependence, the unphysical properties not shared by the true (unknown) sum. The approximant $\sqrt{\mathcal{A}_{S^2}}$, however, possesses RScl and RSch independence, and is thus better suited to bring us closer to the true sum.

On the other hand, when compared with the structure of the ECH and TPS-PMS approximants, $\sqrt{\mathcal{A}_{S^2}}$ possesses a theoretically favorable ‘‘PA type’’ feature that the other two methods do not have: It represents an efficient quasianalytic continuation of the NNLO TPS $S_{[2]}$ from the perturbative (small- a) to the nonperturbative (large- a) regime. This is so because $\sqrt{\mathcal{A}_{S^2}}$ is related with the mentioned DPA method $[2/2]_{S^2}^{1/2}$ (see above). The ECH and the TPS-PMS approximants do not possess this strong type of mechanism of quasianalytic continuation, because they do not go beyond the polynomial TPS structure of the original TPS $S_{[2]}$. These two approximants do possess, however, a weaker type of quasianalytic continuation mechanism, provided by the RGE evolution of the coupling parameter a itself. In the one-loop limit, this would amount to the $[1/1]$ PA-type quasianalytic continuation mechanism for a itself, which may explain why especially the ECH method appears to do well even in the deep nonperturbative regime (where S has large values).

The possibility to adjust the value of the $N^3\text{LO}$ coefficient r_3 of Eq. (36) by the IR_1 pole requirement $y_{\text{pole}} (\equiv 2\beta_0 z) = 2$ in the BPSR was suggested by the authors of Ref. [36]. They chose r_3 (at $\text{RScl } Q_0^2 = Q_{\text{ph}}^2$ and in $\overline{\text{MS}}$ RSch) approximately so that the PA $[2/1]$ of the simple Borel transform of that TPS gave $y_{\text{pole}} \approx 2$. In fact, they chose $r_3 = 130.0$, which would correspond to their $y_{\text{pole}} \approx 2.10$, and then resummed the obtained $N^3\text{LO}$ TPS for $S(Q_{\text{ph}}^2 = 3 \text{ GeV}^2)$ by the $[2/2]$ DPA. However, as we argued in the paragraph following Eq. (47), a procedure involving the simple (RScl- and RSch-dependent) Borel transform leads in general to resummed predictions which can have significant dependence on the RScl and RSch used in the original TPS (including $c_3^{(0)}$ dependence). Their approach (with $r_3 = 130.0$ and $[2/2]$ DPA) would result in $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2) = 0.2934_{-0.0370}^{+0.0276}$ for case I, and $0.2891_{-0.1058}^{+0.0549}$ for case II; and $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.1202_{-0.0062}^{+0.0040}$ for case I and $0.1140_{-0.0201}^{+0.0068}$ for case II. Comparing with results in Table II, we see that these predictions are again very close to the predictions of $[2/2]_{S^2}^{1/2}$, the latter being based solely on the NNLO TPS (36). Recently, in the context of the Borel-Padé method of resummation (not used here), the knowledge of the location of renormalon poles was used in Ref. [44], in two physical examples, to fix the denominator structure of the PA’s of the Borel transform.

V. BPSR: USING PADÉ-RESUMMED β FUNCTIONS

Since nonperturbative physics appears to be of high relevance for the high-precision predictions in the case of the considered observable, one may go still one step further. Until now, we used for the β functions appearing in the integrated RGE (41) [see also Eq. (3)] simply their TPS to the known order

$$\text{TPS}_\beta(x) = -\beta_0 x^2 (1 + c_1 x + \bar{c}_2 x^2 + \bar{c}_3 x^3), \quad (59)$$

where $x \equiv \alpha_s / \pi$, and the bar over symbols denotes that they are different in different RSch’s. However, in the nonperturbative region of large x , these TPS’s may give wrong numerical results. To address this question, we may instead

construct PA’s based on these TPS’s. PA’s represent approximate analytic continuations (i.e., quasianalytic continuations) for the true $\beta(x)$ functions from the perturbative (small- x) into the nonperturbative (large- x) region. A comprehensive source on mathematical properties of PA’s is the book [45]. We have for Eq. (59) three PA candidates: $[2/3]_\beta$, $[3/2]_\beta$, and $[4/1]_\beta$. Constructing these PA’s on the basis of the TPS (59), and then reexpanding in powers of x , gives us the higher order RSch parameters c_j ($j \geq 4$) that were up until now simply set equal to zero. Only our approximant $\sqrt{\mathcal{A}_{S^2}}$, and the ECH and TPS-PMS approximants for the NNLO TPS’s (2), are sensitive to this change. Predictions $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ of Padé resummation approximants for $S(Q_{\text{ph}}^2)$ in the previous section, and the TPS evaluations themselves (NNLO, $N^3\text{LO}$), are not affected by this change (they were calculated in $\overline{\text{MS}}$ RSch and at RScl $Q_0^2 = Q_{\text{ph}}^2$, $n_f = 3$).

For the approximant $\sqrt{\mathcal{A}_{S^2}}$ the relevant RSch’s are those of a_1 (RSch1) and a_2 (RSch2), i.e., those with the RSch parameters $(c_2^{(1)}, c_3, \dots)$ and $(c_2^{(2)}, c_3, \dots)$, where the ellipses stand for $c_k^{(1)}$ and $c_k^{(2)}$ ($k \geq 4$) as determined by our choice of PA for the RSch1 and RSch2 β functions, respectively. Analogously, for the ECH and TPS-PMS approximants, the RSch’s are (ρ_2, c_3, \dots) and $(3\rho_2/2, c_3, \dots)$, where the dots stand for those RSch parameters determined by our choice of the PA for the ECH and TPS-PMS β functions. So, each of the three choices of the PA defines, by the aforementioned mechanism of quasianalytic continuation into the nonperturbative sector, the unique schemes RSch1, ECH RSch, TPS-PMS RSch, and $\overline{\text{MS}}$.

For RSch2, we have to keep in mind one detail: In order to avoid presumably unnecessary complications, the PMS conditions (B1),(B2) were written and used for the choice $c_4^{(2)} = c_4^{(1)}$ ($\delta c_4 = 0$), so that the solutions (39),(40) for Q_1 , Q_2 , $c_2^{(1)}$, and $c_2^{(2)}$ were independent of $c_3 (= c_3^{(1)} = c_3^{(2)})$ and of all the other $c_k^{(j)}$ ($k \geq 4$; $j = 1, 2$). Therefore, once we choose a specific $[M/N]_\beta$ of the RSch1, the predicted c_4 must be reproduced also by the $[M'/N']_\beta$ of the RSch2. This means that the order of the latter PA is by one unit higher than that of the former: $M' + N' = M + N + 1$. Since the PA choices for the RSch1 β function are $[2/3]$, $[3/2]$, and $[4/1]$, those for the RSch2 β function are $[2/4]$, $[3/3]$, $[4/2]$, $[5/1]$. As to the numerics, the situation does not change much when different choices of $[M'/N']_\beta$ or even TPS for the RSch2 are taken (with $c_4^{(2)} = c_4^{(1)}$, and always the same fixed value of c_3). This is so because, in the strong-coupling regimes $S \geq 0.155$, a_1 is by a factor of 1.66 or more larger than a_2 . Concerning the choice of PA_β of $\overline{\text{MS}}$ RSch, this choice does not influence the predictions of c_3 at all, and influences only little the subsequent predictions for $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$. The latter is true mainly because of the hierarchy $a_0 < a_2 < a_1$ ($Q_0 > Q_2 > Q_1$: $Q_1 \approx 0.343 Q_{\text{ph}}$, $Q_2 \approx 0.672 Q_{\text{ph}}$, $Q_0 = Q_{\text{ph}} \approx 1.73$, or 2.24 GeV).

For the various PA_β choices of RSch1, RSch2, ECH RSch, and TPS-PMS RSch, we can just redo the entire calculation of the invariant Borel transforms \bar{B}_S of Eq. (50) and of their PA’s, and find predictions for c_3 that give us the

TABLE III. As in Table I, but the β functions in the approximants are taken as $[2/3]_\beta$ (RSch1), $[2/4]_\beta$ (RSch2; $c_4^{(2)}=c_4^{(1)}$); $[3/2]_\beta$ (ECH RSch, and TPS-PMS RSch).

$PA_{\bar{\beta}}$	c_3 for $\sqrt{\mathcal{A}}$: $[2/3]_{\beta 1}, [2/4]_{\beta 2}$	c_3 for ECH: $[3/2]_\beta$	c_3 for TPS-PMS: $[3/2]_\beta$
[2/1]	21.7	35.1	35.1
[3/1]	15.7	22.9	21.5
[4/1]	15.8	20.8	18.7
[5/1]	16.9	19.6	17.3
[1/2]	12.8	17.3	17.3
[2/2]	14.9	20.4	19.4
[3/2]	15.8	$20.7 \pm 2.8i$	$17.3 \pm 3.6i$
[4/2]	15.7	$20.4 \pm 1.8i$	$17.0 \pm 2.6i$
[1/3]	15.0	20.6	19.5
[2/3]	$15.1 \pm 1.2i$	19.3	18.5
[3/3]	$14.0 \pm 1.7i$	$20.2 \pm 2.0i$	$16.9 \pm 2.7i$
average	≈ 15.5	≈ 20.0	≈ 19.0

correct IR₁ pole $y_{\text{pole}}=2$. It turns out that the most stable c_3 predictions in our approximant $\sqrt{\mathcal{A}}_{S^2}$ are those with $[2/3]_{\beta 1}$ for RSch1 ($\beta 1$) and $[2/4]_{\beta 2}$ for RSch2 ($\beta 2$). The choice $[2/3]_{\beta 1}$ and $[5/1]_{\beta 2}$ gives virtually the same and almost as stable predictions for c_3 . For the ECH and TPS-PMS approximants, all three choices $[2/3]_\beta$, $[3/2]_\beta$, and $[4/1]_\beta$ give comparably stable and mutually quite similar c_3 predictions, but the choice $[3/2]_\beta$ seems to be slightly more stable than the other two. The results, for the mentioned optimal choices of $PA_{\bar{\beta}}$'s for the three approximants, are given in Table III, in complete analogy with Table I. In some cases there are also other solutions for c_3 , not included in the table, which differ significantly from those given in the table. We will adopt the approximate predictions as suggested by $PA_{\bar{\beta}}$'s of intermediate orders ($[3/1]$, $[4/1]$, $[2/2]$, $[3/2]$, $[1/3]$, $[2/3]$): $c_3 \approx 15.5$ for $\sqrt{\mathcal{A}}_{S^2}$; $c_3 \approx 20$ for the ECH; $c_3 \approx 19$ for the TPS-PMS. The actual values of c_3 must be exactly real.

We recall that the results of the previous two sections, including those of Table I, were for the simple choice of TPS_β (59) for the corresponding RSch's ("truncated RSch's," with $c_k=0$ for $k \geq 4$). Comparing those results with the results of Table III, we see that the latter are somewhat higher and significantly more stable under the change of the choice of $PA_{\bar{\beta}}$. This latter fact can be regarded as a numerical indication that it makes sense to use certain PA resummations for the pertaining β functions of approximants when the considered observable (in this case BPSR) contains nonperturbative effects.

When the order of $PA_{\bar{\beta}}$ is increased, the trend of the predictions is similar as in Table I: The predictions c_3 tend to stabilize at intermediate orders of the $PA_{\bar{\beta}}$'s. The lowest order $PA_{\bar{\beta}}$'s ($[1/2]$, and above all $[2/1]$) give unreliable predictions for c_3 , apparently because of a too simple structure of these PA's. The highest order $PA_{\bar{\beta}}$'s ($[5/1]$, $[4/2]$, $[3/3]$) also sometimes give unreliable predictions, apparently because of their "overkill" capacity—these $PA_{\bar{\beta}}$'s depend on many terms in the power expansion of the approximant (up to $\sim \tilde{a}^7$), while the original TPS (36) on which the approxi-

mant is based is given only up to $\sim a_0^3$ ($\sim \tilde{a}^3$). Therefore, it seems plausible that the best and most stable predictions are given by $PA_{\bar{\beta}}$'s of intermediate orders ($[3/1]$, $[4/1]$, $[2/2]$, $[3/2]$, $[1/3]$, $[2/3]$).

With these choices for the values of c_3 and for the pertaining β functions, we could now go on to calculating predictions of the three approximants for $\alpha_s^{\overline{\text{MS}}}$. Since the choice of PA_β for $\overline{\text{MS}}$ RSch will not matter much numerically, as we argued above, we could just choose blindly a PA_β or even the TPS for it. But at this point, we want to point out an additional argument for the made PA_β choices of RSch1/RSch2, ECH RSch, and TPS-PMS RSch. This argument will, in addition, lead us to a specific choice of PA_β for $\overline{\text{MS}}$ RSch.

In this context, we recall first that quasianalytic continuation, e.g., via PA's, of the TPS of a β function into the large- x (nonperturbative) region leads in general to a pole of such $PA_\beta(x)$ at some positive x . The authors of Ref. [46] pointed out that these poles "suggest the occurrence of dynamics in which both a strong and an asymptotically free phase share a common infrared attractor." Now, if there is such a common point $x_{\text{pole}} \equiv \alpha_s^{\text{pole}}/\pi$ where the two phases meet, it is reasonable to expect that its numerical value does not vary wildly when we change RSch—provided that the RSch's in question are themselves physically motivated (physically reasonable) in the nonperturbative regime.¹¹ Such physically motivated RSch's should include those connected in some significant way with the calculation of the considered observable and of the predicted coupling parameters. In the case of our approximant $\sqrt{\mathcal{A}}_{S^2}$, these are RSch1 and RSch2, and in addition $\overline{\text{MS}}$ when we want to extract $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ from the approximant. In Fig. 2 we present the TPS's of RSch1, RSch2 and $\overline{\text{MS}}$ β functions, as well as the previously chosen $[2/3]_{\beta 1}$ of RSch1 and $[2/4]_{\beta 2}$ of RSch2 (see Table III; $c_3=15.5$), and we include also $[2/3]_\beta$ of $\overline{\text{MS}}$ RSch. The figure shows that all these PA β functions have about the same x_{pole} ($x_{\text{pole}}=0.334, 0.325, 0.311$, respectively). The mutual proximity of x_{pole} 's of RSch1 and RSch2 $PA_{\bar{\beta}}$'s is now yet another indication that these $PA_{\bar{\beta}}$'s, chosen previously on the basis of the stability of c_3 predictions, are the reasonable ones. Further, $[2/3]_\beta$ appears to be the reasonable choice for $\overline{\text{MS}}$ RSch. The choices $[3/2]_\beta$ and $[4/1]_\beta$ for $\overline{\text{MS}}$ RSch give $x_{\text{pole}}=0.119, 0.213$, respectively, which is further away from the x_{pole} of RSch1 and RSch2. We could choose, in principle, for RSch1 and RSch2 other $PA_{\bar{\beta}}$'s. We recall that for RSch1 we can have: $[2/3]_{\beta 1}$, $[3/2]_{\beta 1}$, $[4/1]_{\beta 1}$; for RSch2: $[2/4]_{\beta 2}$, $[3/3]_{\beta 2}$, $[4/2]_{\beta 2}$, $[5/1]_{\beta 2}$. However, when taking $[3/2]_{\beta 1}$ or $[4/1]_{\beta 1}$, we always end up either with a situation when the two positive x_{pole} values of $\beta 1$ and $\beta 2$ are far apart, or both are unphysically small, or one positive x_{pole} does not exist, or there are virtually no predictions for c_3 (not even unstable ones), or x_{pole} values are very unstable under the change of c_3 in the interesting region $c_3 \approx 12-16$. Concerning the latter point—when taking $[3/2]_{\beta 1}$, and for RSch2

¹¹In the perturbative regime, all RSch's are formally equivalent.

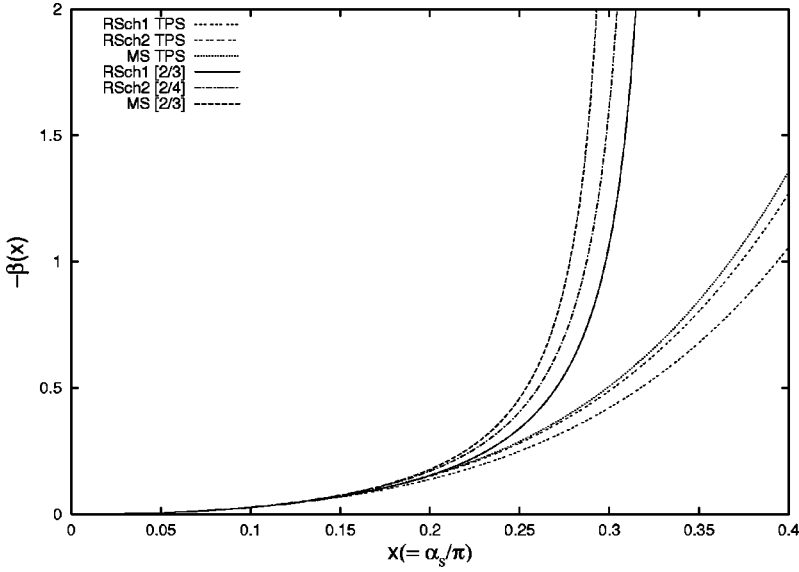


FIG. 2. TPS β functions for RSch1 and RSch2 ($c_3=15.5$), and $\overline{\text{MS}}$ ($n_f=3$), and their corresponding PA's $[2/3]$, $[2/4]$ ($c_4^{(2)}=c_4^{(1)}$), and $[2/3]$, respectively.

$[3/3]_{\beta_2}$ or $[4/2]_{\beta_2}$, the location of x_{pole} of the latter PA_{β} 's changes drastically when c_3 is varied around the interesting values of 12–16, thus signalling instability of these PA_{β} 's. The choice $[2/3]_{\beta_1}$ and $[5/1]_{\beta_2}$, which gave very similar and almost as stable results for c_3 as the most preferred choice $[2/3]_{\beta_1}$ and $[2/4]_{\beta_2}$, gives the corresponding poles again close to each other: $x_{\text{pole}}=0.334, 0.291$, respectively. So, the PA_{β} choices $[2/3]_{\beta_1}$ and $[2/4]_{\beta_2}$ (or $[5/1]_{\beta_2}$) for our approximant give us the most stable c_3 predictions and are the only ones giving mutually similar (and reasonable) values of x_{pole} of RSch1 and RSch2.

It is also encouraging that the choices $[3/2]_{\beta}$ for the ECH and TPS-PMS RSch's give us x_{pole} values comparable to the ones previously mentioned: $x_{\text{pole}}=0.263$ for ECH with $c_3=20$; $x_{\text{pole}}=0.327$ for TPS-PMS with $c_3=19$. Even other choices of PA_{β} for the ECH and TPS-PMS RSch's ($[2/3]_{\beta}$, $[4/1]_{\beta}$), which also gave rather stable and similar c_3 predictions, give us $x_{\text{pole}} \approx 0.27-0.41$. Hence, also in this case we see correlation between the stability of the c_3 predictions on the one hand and $x_{\text{pole}} \approx 0.3-0.4$ on the other.

The authors of Refs. [47,48] estimated the five-loop coefficient $c_4^{\overline{\text{MS}}}$ of the $\overline{\text{MS}}$ β function, by applying their method of asymptotic Padé approximation (APAP) [47] and its improvement using estimators over negative numbers of flavors (WAPAP) [48]. Their predicted values by two variants of the latter method, when including the four-loop quartic Casimir contributions, are $c_4^{\overline{\text{MS}}}=123.7, 115.3$ (see Tables III and IV in Ref. [48], respectively; $n_f=3$). On the other hand, the simple PA's $[2/3]$, $[3/2]$, $[4/1]$ for $\overline{\text{MS}}$ β function predict $c_4^{\overline{\text{MS}}}=62.2, 149.8, 98.5$, and $x_{\text{pole}}=0.311, 0.119, 0.213$, respectively. If we assume that the actual value of $c_4^{\overline{\text{MS}}}$ is close to the one predicted by Ref. [48], and if we were led just by the requirement that the PA should reproduce well this value, then $[4/1]$ would be the preferred choice. However, the authors of Ref. [48] indicated that their predicted value of c_4 may be changed significantly if new Casimir terms, appearing for the first time at the five-loop order, are large. Our choice $[2/3]$ for $\overline{\text{MS}}$ β function was motivated by the value

of $x_{\text{pole}}=0.311$ lying close to x_{pole} of the β functions appearing in the discussed approximants for the BPSR. Further, the precise choice of the PA for $\overline{\text{MS}}$ β function practically does not influence the numerical results of our analysis, because $a_0 \equiv a(\ln Q_{\text{ph}}^2; c_2^{\overline{\text{MS}}}, \dots)$ is significantly smaller than the coupling parameters $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, c_4, c_5^{(j)}, \dots)$ ($j=1,2$) appearing in our approximant, and the parameters a_{ECH} and a_{PMS} appearing in the ECH and the TPS-PMS approximants.

To summarize, the best choice in calculating $\alpha_s^{\overline{\text{MS}}}$ from our approximant $\sqrt{\mathcal{A}_{S^2}}$ is $c_3 \approx 15.5$, the PA_{β} choice $[2/3]_{\beta}$ for RSch1, $[2/4]_{\beta}$ choice for RSch2 ($c_4^{(2)}=c_4^{(1)}$), and $[2/3]_{\beta}$ for $\overline{\text{MS}}$ RSch; the best choice in calculating $\alpha_s^{\overline{\text{MS}}}$ from the ECH and TPS-PMS approximants is $c_3 \approx 20$ and 19, respectively, the PA_{β} choice $[3/2]_{\beta}$ for ECH RSch and TPS-PMS RSch; and $[2/3]_{\beta}$ for $\overline{\text{MS}}$ RSch; our, the ECH and the TPS-PMS approximants are completely independent of the original choice of the RSch and RSch, because the c_3 parameter is determined by using the RSch or RSch invariant Borel transform $\overline{B}(z)$ of Sec. III.

In practice, this means that for our approximant $\sqrt{\mathcal{A}_{S^2}}$ the two coupling parameters $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, c_4, c_5^{(j)}, \dots)$ ($j=1,2$) are now related with the coupling parameter $a_0 \equiv a(\ln Q_0^2; c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}}, c_4^{\overline{\text{MS}}}, \dots)$ via the following (PA-)version of the subtracted Stevenson equation (41) [see also Eqs. (A1)–(A2)]:

$$\begin{aligned} \beta_0 \ln \left(\frac{Q_j^2}{Q_0^2} \right) &= \frac{1}{a_j} + c_1 \ln \left(\frac{c_1 a_j}{1 + c_1 a_j} \right) \\ &+ \int_0^{a_j} dx \frac{\{\text{PA}_{\beta_j}(x) + \beta_0 x^2 (1 + c_1 x)\}}{x^2 (1 + c_1 x) \text{PA}_{\beta_j}(x)} \\ &- \frac{1}{a_0} - c_1 \ln \left(\frac{c_1 a_0}{1 + c_1 a_0} \right) \\ &- \int_0^{a_0} dx \frac{\{[2/3]_{\text{MS}\beta}(x) + \beta_0 x^2 (1 + c_1 x)\}}{x^2 (1 + c_1 x) [2/3]_{\text{MS}\beta}(x)}, \end{aligned} \quad (60)$$

TABLE IV. Predictions for $\alpha_s^{\overline{\text{MS}}}$ for our, ECH, and TPS-PMS approximants, when the PA-resummed β functions in the approximants are taken as in Table III. Predictions for case I (53) and case II (52) are given in parallel.

Approximant (with PA $_{\beta}$'s)	$\alpha_s(5 \text{ GeV}^2)$: (I)	$\alpha_s(3 \text{ GeV}^2)$: (II)	$\alpha_s(M_Z^2)$: (I)	$\alpha_s(M_Z^2)$: (II)
$\sqrt{\mathcal{A}_{S^2}^{[2/2]}} (c_3 = 15.5)$	$0.2838^{+0.0182}_{-0.0311}$	$0.2805^{+0.0297}_{-0.0977}$	$0.1187^{+0.0028}_{-0.0054}$	$0.1127^{+0.0041}_{-0.0189}$
ECH ($c_3 = 20.0$)	$0.2856^{+0.0195}_{-0.0321}$	$0.2822^{+0.0325}_{-0.0993}$	$0.1190^{+0.0030}_{-0.0056}$	$0.1130^{+0.0044}_{-0.0192}$
TPS-PMS ($c_3 = 19.0$)	$0.2867^{+0.0202}_{-0.0328}$	$0.2831^{+?}_{-0.1001}$	$0.1192^{+0.0030}_{-0.0057}$	$0.1131^{+?}_{-0.0192}$

where PA $_{\beta_j}$ stands for the mentioned $[2/3]_{\beta}$ of RSch1 (when $j=1$) and $[2/4]_{\beta}$ of RSch2 (when $j=2$), with $c_3 = 15.5$. We recall that the scales Q_j^2 and the parameters $c_2^{(j)}$ ($j=1,2$) of the approximant, which are RScI- and RSch-invariant and calculated in Secs. II and III [see Eqs. (39),(40)], are independent of the parameter c_3 and of any higher order β parameter $c_k^{(j)}$ ($k \geq 4$; $j=1,2$) appearing in $a_j \equiv a(\ln Q_j^2; c_2^{(j)}, c_3, c_4, c_5^{(j)}, \dots)$. For the ECH and TPS-PMS the calculation is performed in an analogous way.

The results of these calculations, i.e., the predicted values of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ and $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$, are given in Table IV for the approximants $\sqrt{\mathcal{A}_{S^2}}$, ECH and TPS-PMS. The predictions are now a little, but still significantly, lower than those of the corresponding approximants in Table II where all the β functions were taken in the TPS form (59) and with $c_3 = 12.5, 17, 16$, respectively. The evolution from $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ to $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ was performed as in the previous section, i.e., with the four-loop RGE (i.e., TPS β function of $\overline{\text{MS}}$) and the correspond-

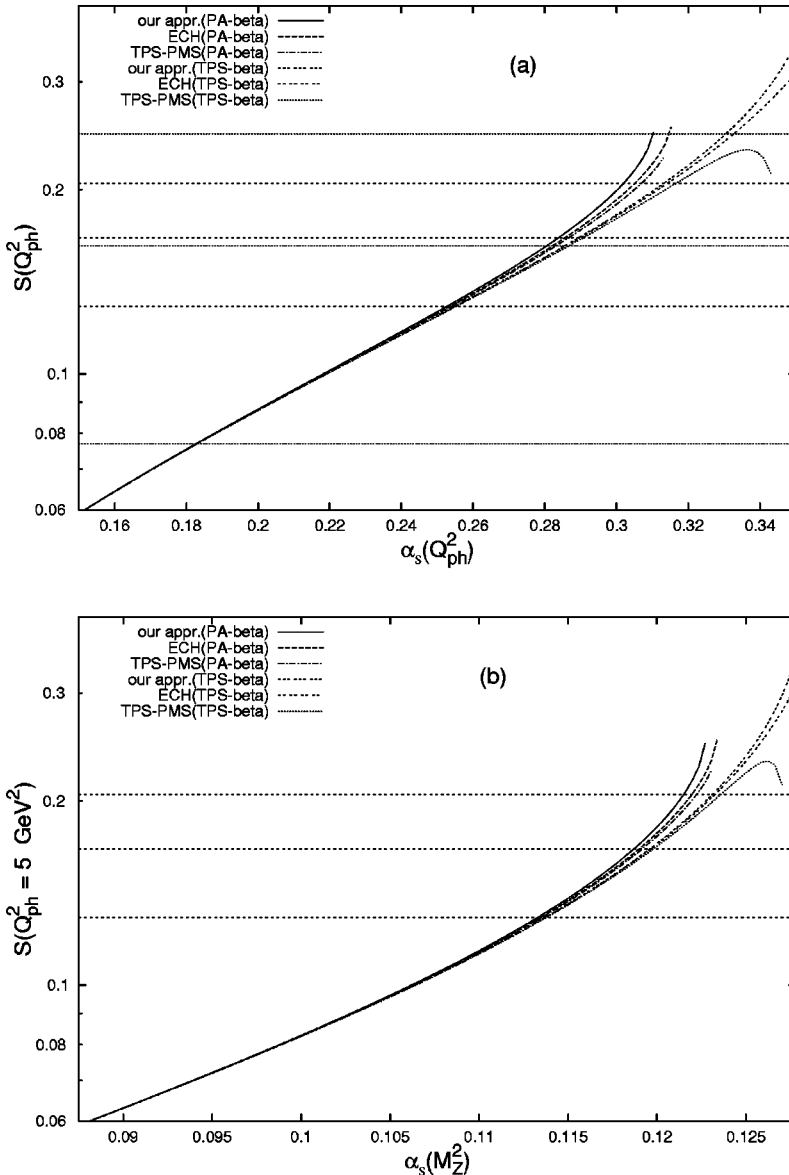


FIG. 3. Predictions of our approximant (with $c_3 = 15.5$), ECH (with $c_3 = 20.0$), and TPS-PMS (with $c_3 = 19.0$): (a) for $S(Q_{\text{ph}}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ when $n_f=3$; (b) for $S(Q_{\text{ph}}^2 = 5 \text{ GeV}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$. The PA choices of the RGE β functions were made as explained in the text. For comparison, we include also the corresponding predictions from Figs. 1 when the TPS's (59) are used for the β functions. The values of the c_3 parameter have been adjusted in all cases to ensure the correct location of the leading IR renormalon pole. The experimental bounds are denoted as in Fig. 1.

ing three-loop flavor threshold matching conditions. If we replace the TPS β function of $\overline{\text{MS}}$ by its PA $[2/3]_\beta$ in the RGE for the evolution $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2) \mapsto \alpha_s^{\overline{\text{MS}}}(M_Z^2)$, the results for $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ decrease insignificantly (by less than 0.04%) and the numbers in Table IV do not change.

In Fig. 3(a) we present predictions $S(Q_{\text{ph}}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ ($n_f=3$, e.g. $Q_{\text{ph}}^2=3$ or 5 GeV^2), and in Fig. 3(b) the predictions for $S(5 \text{ GeV}^2)$ as functions of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$, for the three approximants with the aforementioned PA choices for the β functions. For comparison, we include in the figures also predictions of these three approximants when all the β functions have the TPS form (59) and the correspondingly smaller c_3 's (the latter curves are contained also in Fig. 1). Predictions of the PA resummation approximants (for S) are not included, since these methods are insensitive to the mentioned PA quasianalytic continuation of the β functions and the results remain for them the same as in Figs. 1 and Table II. We presented in Figs. 3 the curves for the case of approximants with the mentioned PA β functions only so far as the method works. More specifically, when the integration interval in the first integral of Eq. (60) starts including values x larger than those at which the absolute value of the PA_β exceeds the value 2, we stop the calculation of the approximant since the latter would otherwise probe values too near the pole of PA_β (i.e., too near the common point of the asymptotically free and the strong phase) and would thus be unreliable.

The considered BjPSR observable $S(Q_{\text{ph}}^2)$ has a higher-twist (HT) contribution, estimated from QCD sum rule [49]¹²

$$S^{(\text{HT})}(Q_{\text{ph}}^2) \approx \frac{(0.09 \pm 0.045) \text{ GeV}^2}{Q_{\text{ph}}^2}, \quad (61)$$

which should be added to the perturbation series for S . If adding this term in the numerical analysis, the predicted central values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ given in Table II decrease significantly. For example, the NNLO TPS central value predictions $\alpha_s^{\overline{\text{MS}}}(M_Z^2)=0.1252$ (case I) and 0.1183 (case II) then decrease to 0.1200 – 0.1236 (case I) and 0.1091 – 0.1157 (case II), where the lower and upper values in each case correspond to the largest and the smallest value choice in Eq. (61). This indicates numerically that our approximant ($c_3=15.5$, Table IV), which gives the central values $\alpha_s^{\overline{\text{MS}}}(M_Z^2)=0.1187$ (case I) and 0.1127 (case II), already contains at least part of the nonperturbative effects from the leading higher-twist operator ($\sim 1/Q_{\text{ph}}^2$). The same is true for the ECH ($c_3=20.0$) and TPS-PMS ($c_3=19.0$). In order to understand this numerical indication, we recall that the information on the location of the leading IR renormalon (IR_1) pole of the considered observable has already been incorporated in these approximants, via the aforementioned fixing of the value of the c_3 parameter. And the so called ambiguity of

the leading IR renormalon is of the same form $\sim 1/Q_{\text{ph}}^2$ as the higher-twist term (61), and even the estimated coefficients are of the same order of magnitude [51] (see also Ref. [36] on this point). Our approximant, the ECH and the TPS-PMS, via the discussed c_3 fixing, implicitly provide approximant-specific prescriptions of how to integrate in the Borel integral over the IR_1 pole, thus eliminating the (leading) renormalon ambiguity.

VI. DISCUSSION OF THE NUMERICAL RESULTS

The main reason to apply our approach (and PA approaches) to the BPSR was to investigate efficiencies of various methods and the influence of the nonperturbative sector. Another reason was that the BPSR is a Euclidean observable ($q_{\text{ph}}^2 = -Q_{\text{ph}}^2 < 0$), and for such observables various resummation methods are believed to work well since no real particle thresholds are involved in the observable [52,53].

The main prediction of our approximant $\sqrt{\mathcal{A}_{S^2}}$ can be read off from Table IV, for two cases (53) and (52) of the BPSR-integral values at $Q_{\text{ph}}^2=5$ and 3 GeV^2 , respectively, extracted from experiments

$$\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.1187_{-0.0054}^{+0.0028} \quad (\text{I}); \quad 0.1127_{-0.0189}^{+0.0041} \quad (\text{II}). \quad (62)$$

The ECH and the TPS-PMS give results similar to these, when the c_3 parameter in them is adjusted in the aforementioned way—see Table IV. The diagonal PA (DPA) methods give higher predictions, and the nondiagonal PA methods even higher—see Table II and Fig. 1.

The result (62) for case II, which is based on the measurements before 1997 and a NLO PQCD extrapolation for low x_{Bj} [37] (52), shows quite large uncertainties, a consequence of the large uncertainties (56) [(52)]. The result (62) for case I, based on the most recent measurements and a similar NLO PQCD extrapolation for small x_{Bj} , by the SLAC E155 Collaboration [19] (53), already shows significantly reduced uncertainties. This is so to a large degree because of additional new measurements in the low- x_{Bj} regime. And most importantly, the central values of case I in Eq. (62) are now significantly higher than those of (the older) case II. We recall that the central values in Eq. (62) correspond to the central values of the BPSR integral (53) and (52). We did not attempt to estimate the theoretical uncertainties originating from the resummation method itself. However, the combined results of Table IV $\alpha_s^{\overline{\text{MS}}}(M_Z^2)=0.119_{-0.006}^{+0.003}$ for (new) case I could be regarded as containing nonconservatively estimated theoretical uncertainties.

The present world average is $\alpha_s^{\overline{\text{MS}}}(M_Z^2)=0.1173 \pm 0.0020$ by Ref. [54], and 0.1184 ± 0.0031 by Ref. [55]. Predictions of the simple (NNLO) TPS evaluation in (new) case I give $0.1252_{-0.0078}^{+0.0055}$ (see Table II), the central value and most of the interval lying significantly above the world average. On the other hand, the simple (NNLO) TPS evaluation in (older) case II predicts $0.1183_{-0.0232}^{+0.0095}$ (see Table II), the central value agreeing well with the world average, but the uncertainty interval being much broader. However, the situ-

¹²Deficiencies of the QCD sum rule calculations were pointed out in Ref. [50].

ation changes drastically when employing more sophisticated resummation methods. The values for BPSR-predicted $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ go down the more significantly, the more sophisticated resummation we perform—see Table II for the PA methods, and for TPS-PMS, ECH, and $\sqrt{\mathcal{A}_{S^2}}$ when the β functions have truncated form, and Table IV for the last three methods when the β functions are resummed. The predictions of approximants in the latter table have $\alpha_s^{\overline{\text{MS}}}(M_Z^2) \approx 0.119_{-0.006}^{+0.003}$ (case I, new) and $0.113_{-0.019}^{+0.004}$ (case II, old). The predictions of (new) case I now agree well with the world average 0.1184 ± 0.0031 of Ref. [55], while those of (older) case II lie almost entirely below the world average intervals.

Thus, the use of resummation methods which account for nonperturbative contributions by the mechanism of quasianalytic continuation and by incorporation of the information on the leading IR renormalon pole, predict the values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ which agree well with the present world average if the most recent BPSR data [19] are used. This suggests, among other things, that for reliable predictions of $\alpha_s^{\overline{\text{MS}}}$ from reasonably well measured low-energy QCD observables, we have to know the NNLO terms ($\sim a^3$), employ nontrivial resummation methods, and possibly incorporate some nonperturbative (renormalon) information in the resummation.

Some of the recently performed analyses beyond the NLO, by other authors, gave predictions $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.118 \pm 0.006$ [56] from the CCFR data for $x_{\text{Bj}}F_3$ structure function from νN deep inelastic scattering (DIS) (NNLO); 0.1172 ± 0.0024 [57] from IN DIS (NNLO); 0.115 ± 0.008 [58]; and $0.114_{-0.012}^{+0.010}$ [59] from the Gross-Llewellyn-Smith sum rule (NNLO); 0.1181 ± 0.0031 from hadronic τ decay (NNLO, combined results, [55]); 0.115 ± 0.004 [60,54] from lattice computations.

We note that the BPSR predictions deviate from the world average in case I' (54), i.e., when we include in the experimental data of case I the nuclear effects originating from spin-one isosinglet 6-quark clusters in deuteron and helium according to Ref. [41], on top of the nuclear wavefunction effects and NLO PQCD small- x_{Bj} extrapolation effects: $\alpha_s^{\overline{\text{MS}}}(M_Z^2) \approx 0.103_{-0.027}^{+0.014}$ (NNLO TPS); $0.101_{-0.025}^{+0.013}$ (DPA, ECH, TPS-PMS, our approximant). The combination of (older) case II results and the mentioned 6-quark cluster nuclear effects (case II') increases the value of the BPSR integral so much that the predicted values of $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$ are unacceptably low: the central values would be 0.094–0.095 for all approximants; the maximal allowed values would be about 0.113 by the methods of Table IV and 0.114 by the DPA.

The authors of Ref. [37] obtained, among other things, the BPSR-predicted values $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.118_{-0.026}^{+0.010}$, apparently using the simple NNLO TPS sum (36) directly in their analysis. They used the BPSR-integral values (52), i.e., here case II, which were extracted by them from low- Q_{ph}^2 SLAC experiments carried out before 1997. They used the value of $|g_A| = 1.257$ known at the time, in contrast to the value of Eq. (38). Their RGE evolution from $Q_{\text{ph}}^2 = 3 \text{ GeV}^2$ to M_Z^2 was apparently carried out at the three-loop level, since the fourth-loop β coefficient $c_3^{\overline{\text{MS}}}(n_f)$ [42] and the corresponding

three-loop flavor-threshold matching [53] were not known at the time. These two effects largely neutralize each other and their result is then close to the NNLO TPS result for case II (Table II): $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.118_{-0.023}^{+0.010}$.

The authors of Ref. [36] obtained the BPSR-predicted values $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.116_{-0.005}^{+0.003} \pm 0.003$. They used a DPA method of resummation $[2/2]_S$ mentioned towards the end of Sec. IV. However, they took the BPSR-integral values (51) where the naive Regge small- x_{Bj} extrapolation was used, and apparently the value $|g_A| = 1.257$ known at the time. Further, they included the effects of the higher-twist term (61) on top of their DPA resummation. The additional uncertainty ± 0.003 can be called the method uncertainty. It was estimated by them by additionally using the results of the non-diagonal PA resummations $[1/2]_S$ and $[2/1]_S$, the RScl dependence of their DPA results, and the uncertainty of the higher-twist term.

When we reexpand the approximants in powers of the original a_0 (at RScl $Q_0^2 = Q_{\text{ph}}^2$, in MS RSch, $n_f = 3$), we obtain predictions for coefficient r_3 at a_0^4 of expansion (36)—cf. Eq. (47) and the discussion following it. Our approximant, with $c_3 = 15.5$, predicts $r_3 = 125.8 - c_3^{\overline{\text{MS}}}/2 + c_3 \approx 130.8$. The ECH approximant, with $c_3 = 20.0$, predicts $r_3 = 129.9 + (-c_3^{\overline{\text{MS}}} + c_3)/2 \approx 129.4$. The two predictions are close to each other, suggesting $r_3 = 130.0 \pm 1$. This agrees well with the prediction of Ref. [52] $r_3 \approx 129.9$ (≈ 130) which was obtained from the ECH under the assumption $(-c_3^{\overline{\text{MS}}} + c_3) \approx 0$ (note that $c_3^{\overline{\text{MS}}} \approx 21.0$ [42] was not even known at the time Ref. [52] was written).

The predictions for r_3 , as well as the values of Q_1^2 , Q_2^2 , $c_2^{(1)}$, $c_2^{(2)}$ (39),(40) and of c_3 (Tables I, III), are for $n_f = 3$ and are, of course, independent of the specific values for the BPSR integral (53), (52) [(55),(56)] that we subsequently used to obtain values for $\alpha_s^{\overline{\text{MS}}}(M_Z^2)$.

VII. SUMMARY AND OUTLOOK

We presented an extension of our previous method of resummation [15–17] for truncated perturbation series (TPS) of massless QCD observables given at the next-to-next-to-leading order (NNLO). While the previous method, partly related to the method of the diagonal Padé approximants (DPA's), completely eliminated the unphysical dependence of the sum on the renormalization scale (RScl), the extension presented here eliminates in addition the unphysical dependence on the renormalization scheme (RSch). The dependence on the leading RSch parameter $c_2^{(0)} \equiv \beta_2^{(0)}/\beta_0$ is eliminated by a variant of the method of the principle of minimal sensitivity (PMS). The dependence on the next-to-leading RSch parameter $c_3^{(0)} \equiv \beta_3^{(0)}/\beta_0$ is eliminated by fixing the c_3 value in the approximant so that the correct value of the location of the leading infrared renormalon (IR_1) pole is obtained (by PA's of an RScl- and RSch-invariant Borel transform). Hence, in the approximant we use β functions which go beyond the highest calculated order in the observable (NNLO)—in order to incorporate an important piece of nonperturbative information (IR_1 pole location) which is not

contained in the available NNLO TPS anyway. The results are apparently further improved when we resum those β functions which are relevant for the calculation of the approximant (RSch1 and RSch2 β functions, for a_1 and a_2) and of $\alpha_s^{\overline{\text{MS}}}(Q_{\text{ph}}^2)$ ($\overline{\text{MS}}$ RSch), by judiciously choosing certain PA forms for those β functions.

We applied this method to the Bjorken polarized sum rule (BPSR) at low values of the momentum transfer of the virtual photon $Q_{\text{ph}}^2 = 5$ or 3 GeV^2 . The c_3 fixing by the IR_1 pole location is well motivated in this case, because the contributions of the leading ultraviolet renormalon (UV_1) appear to be sufficiently suppressed in comparison to those of the IR_1 . We compared predictions of our resummation with the values for the BPSR integral (53) and (52) extracted from experiments, and obtained $\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.1187_{-0.0054}^{+0.0028}$ (new case I) and $0.1127_{-0.0189}^{+0.0041}$ (older case II), respectively. Here, the central values 0.1187 and 0.1127 correspond to the central values in Eqs. (53) and (52), respectively. For more discussion on the issue of the experimental values (53) and (52) (cases I, II) we refer to Secs. IV and VI. It is gratifying that the newest available experimental values (53) lead to predictions for $\alpha_s^{\overline{\text{MS}}}$ which agree well with the present world average. The results of Grunberg's method of the effective charge (ECH) and of Stevenson's TPS-PMS method give very similar results (see Table IV) if the c_3 parameter in these methods is fixed by the same aforementioned requirement as in our approximant and PA forms of the pertaining β functions are chosen analogously. The combined result of Table IV, in case I, i.e., with the newest data of Ref. [19], is

$$\alpha_s^{\overline{\text{MS}}}(M_Z^2) = 0.119_{-0.006}^{+0.003}. \quad (63)$$

The DPA methods of resummation of S predict higher values (central values about 0.120 in case I; 0.114 in case II), the nondiagonal PA's even higher (central values about 0.122 in case I; 0.115 in case II), and the NNLO TPS itself the highest values (central value about 0.125 in case I; 0.118 in case II).

We expect that our approximant $\sqrt{\mathcal{A}_{S^2}}$, as well as the ECH and TPS-PMS, produced reliable resummation results for the considered observable, because—via their dependence on c_3 —we can incorporate into them in the aforementioned way important nonperturbative information about the IR_1 pole, and simultaneously achieve full RSch independence. The c_3 dependence in $\sqrt{\mathcal{A}_{S^2}}$, in the ECH and in the TPS-PMS, is very closely related with the sensitivity of these approximants to the details of the corresponding RGE evolution. These details (c_3 terms) in the RGE evolution are numerically more important in the lower-energy regions, i.e., when the relevant energies for the observable are low. Thus, significant c_3 dependence of these approximants signals the relevance of nonperturbative regimes for the observable [see Eqs. (32),(33)]. It then appears natural that the c_3 parameter in these approximants, i.e., the only parameter left free, is made to parametrize the location of the (nonperturbative) IR_1 pole. The (D)PA's, in contrast, possess besides the c_3 dependence also dependence on the leading RSch-parameter c_2 ,

and even on the RSch. Thus, the parameter c_3 in them is not in a special position, and there is more ambiguity as to how to incorporate into the PA's the information about the IR_1 pole.

It appears that the leading higher-twist term contribution to the BPSR ($\sim 1/Q_{\text{ph}}^2$), or a part of it, is implicitly contained in $\sqrt{\mathcal{A}_{S^2}}$, as well as in the ECH and the TPS-PMS, via the aforementioned c_3 fixing. In this context, we point out that the so called renormalon ambiguity arising from the IR_1 of the BPSR has the form $\sim 1/Q_{\text{ph}}^2$, i.e., the form of the leading higher-twist term. Even the coefficients of this term, as estimated by the renormalon ambiguity arguments, are of the same order of magnitude as those predicted (estimated) from QCD sum rule. One can say that the described approaches implicitly give approximate-specific prescriptions for the elimination of the (leading IR) renormalon ambiguity.

Looking beyond the numerical analysis of the BPSR, we wish to stress that in cases of other QCD observables that are (or eventually will be) known to the NNLO, the analogous numerical analyses may give different hierarchies of numerical results. Actual resummation analyses should be performed also for such observables, in order to shed more light on the questions about the relative importance of various kinds of contributions.

The (D)PA methods, when applied directly to the (NNLO) TPS's, are trying to include some nonperturbative contributions through quasianalytic continuation of the TPS from the perturbative (small- a) to the nonperturbative (large- a) region. In the course of this continuation, the pole structure of the Borel transform of the sum may be missed, but some other nonperturbative (but less singular) features of the sum itself may be reproduced well. But our approximant $\sqrt{\mathcal{A}_{S^2}}$ would presumably do at least as good a job as the DPA's in reproducing these latter nonperturbative features. This is so because $\sqrt{\mathcal{A}_{S^2}}$ (14) reduces to the DPA $[2/2]_{S^2}^{1/2}$ in the large- β_0 (one-loop RGE evolution) approximation when thus the full RSch and RSch invariance requirements are abandoned, see discussion following Eqs. (9)–(11). The ECH and the TPS-PMS methods do not possess this strong “ $[2/2]^{1/2}$ PA type” mechanism of quasianalytic continuation, since these two methods fix the RSch and the RSch in the TPS itself without going beyond the (NNLO) polynomial TPS form in a . The ECH, and somewhat less explicitly the TPS-PMS, possess a weaker type of quasianalytic continuation, because the one-loop RGE-evolved $a \equiv \alpha_s/\pi$ (from a_0) is a $[1/1]$ PA of a_0 .

Stated differently, our (NNLO) approximants, from a theoretical viewpoint, combine the favorable feature of the (D)PA's (strong quasianalytic continuation into the large- a regime) with the favorable feature of the TPS-form NNLO approximants ECH and TPS-PMS (full RSch and c_2 independence). The residual RSch dependence (c_3 dependence) in the latter approximants and in our approximant allows us to incorporate into them, often in a well-motivated manner, nonperturbative information on the location of the leading IR renormalon pole, and to achieve in this way simultaneously the full RSch independence as well.

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APPENDIX A: EXPANSION OF THE GENERAL COUPLING a IN POWERS OF a_0

We outline here the derivation of the expansion of QCD coupling $a \equiv a(\ln Q^2; c_2, c_3, \dots)$ ($a = \alpha_s/\pi$) in power series of $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots)$. The starting point is the Stevenson equation (see Ref. [2], first entry, Appendix A) which is obtained by integrating RGE (3):

$$\beta_0 \ln\left(\frac{Q^2}{\tilde{\Lambda}^2}\right) = \frac{1}{a} + c_1 \ln\left(\frac{c_1 a}{1 + c_1 a}\right) + \int_0^a dx \left[\frac{1}{x^2(1 + c_1 x)} - \frac{1}{x^2(1 + c_1 x + c_2 x^2 + c_3 x^3 + \dots)} \right]. \quad (\text{A1})$$

It can be shown that $\tilde{\Lambda}$ here is a universal scale (~ 0.1 GeV) independent of the scale Q and of the scheme parameters c_j ($j \geq 2$). Writing the analogous equation for a_0 , and subtracting the two, we obtain

$$\begin{aligned} \beta_0 \ln\left(\frac{Q^2}{Q_0^2}\right) &= \frac{1}{a} + c_1 \ln\left(\frac{c_1 a}{1 + c_1 a}\right) \\ &+ \int_0^a dx \frac{(c_2 + c_3 x + \dots)}{(1 + c_1 x)(1 + c_1 x + c_2 x^2 + c_3 x^3 + \dots)} \\ &- \frac{1}{a_0} - c_1 \ln\left(\frac{c_1 a_0}{1 + c_1 a_0}\right) - \int_0^{a_0} dx \\ &\times \frac{(c_2^{(0)} + c_3^{(0)} x + \dots)}{(1 + c_1 x)(1 + c_1 x + c_2^{(0)} x^2 + c_3^{(0)} x^3 + \dots)}. \end{aligned} \quad (\text{A2})$$

This equation determines a as function of a_0 . The solution a in form of a power series of a_0 is the Taylor series for function a of multiple arguments $\ln Q^2$ and c_j 's ($j \geq 2$). To obtain this power series, one way would be to find first the derivatives $\partial a / \partial c_j$ [the derivative $\partial a / \partial \ln Q^2$ is already given by RGE (3)]. For this, we take the partial derivative of both sides of the above equation with respect to c_j ($j \geq 2$) and after some algebra we obtain

$$\begin{aligned} \frac{\partial a}{\partial c_j} &= a^2(1 + c_1 a + c_2 a^2 + c_3 a^3 + \dots) \\ &\times \int_0^a \frac{dx x^{j-2}}{(1 + c_1 x + c_2 x^2 + c_3 x^3 + \dots)^2}. \end{aligned} \quad (\text{A3})$$

Expanding the integrand in powers of x and integrating out each term, we obtain the partial derivatives as power series

$$\frac{\partial a}{\partial c_2} = a^3 \left(1 + \frac{c_2}{3} a^2 + \dots \right), \quad (\text{A4})$$

$$\frac{\partial a}{\partial c_3} = \frac{1}{2} a^4 \left(1 - \frac{c_1}{3} a + \dots \right), \quad (\text{A5})$$

$$\frac{\partial a}{\partial c_4} = \frac{1}{3} a^5 + \dots \quad (\text{A6})$$

Repeated application of these equations, as well as of RGE (3) itself, leads us to the following Taylor expansion of a in powers of $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots)$:

$$\begin{aligned} a &= a_0 + a_0^2(-x) + a_0^3(x^2 - c_1 x + \delta c_2) + a_0^4 \left(-x^3 + \frac{5}{2} c_1 x^2 \right. \\ &\quad \left. - c_2^{(0)} x - 3x \delta c_2 + \frac{1}{2} \delta c_3 \right) + a_0^5 \left[x^4 - \frac{13}{3} c_1 x^3 + \left(\frac{3}{2} c_1^2 \right. \right. \\ &\quad \left. \left. + 3c_2^{(0)} + 6\delta c_2 \right) x^2 + (-c_3^{(0)} - 3c_1 \delta c_2 - 2\delta c_3) x \right. \\ &\quad \left. + \left(\frac{1}{3} c_2^{(0)} \delta c_2 + \frac{5}{3} (\delta c_2)^2 - \frac{1}{6} c_1 \delta c_3 + \frac{1}{3} \delta c_4 \right) \right] + \mathcal{O}(a_0^6), \end{aligned} \quad (\text{A7})$$

where we denoted

$$a \equiv a(\ln Q^2; c_2, c_3, \dots), \quad a_0 \equiv a_0(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots), \quad (\text{A8})$$

$$x \equiv \beta_0 \ln \frac{Q^2}{Q_0^2}, \quad \delta c_k \equiv c_k - c_k^{(0)}. \quad (\text{A9})$$

APPENDIX B: EXPLICIT PMS CONDITIONS

Here we will write explicitly the PMS-like conditions (31) in its lowest order ($\sim \bar{a}_0^5$). To do this, we calculate explicitly the derivatives (31) and then expand them in powers of $\bar{a}_0 = a(\ln Q_0^2; c_2 = c_2^{(0)}; c_3; \dots)$ to their lowest nontrivial order.¹³ We assume relation (34), i.e., $\delta c_3 = 0$, and in addition $\delta c_4 (\equiv c_4^{(1)} - c_4^{(2)}) = 0$. Further, we use relations (26), (27) and notations (28)–(30). The results, obtained with help of MATHEMATICA, are the following:

¹³In fact, a with any RScl and any RSch parameters would do the job and give the same coefficient at the leading nontrivial order a^5 .

$$\left. \frac{\partial \mathcal{A}_{\bar{S}}^{[2/2]}}{\partial c_2^{(s)}} \right|_{\delta c_2} \equiv -\bar{a}_0^5 \{27(\delta c_2)^3 - 157c_1(\delta c_2)^2 y_- - 8\delta c_2 y_-^2 [-27c_1^2 + 12c_2^{(s)} + 34y_-^2 - 8z_0^2(c_2^{(s)})] + 48c_1 y_-^3 [13y_-^2 - 3z_0^2(c_2^{(s)})]\} \{6y_-^2 [5c_1 \delta c_2 + 16y_-^3 - 8z_0^2(c_2^{(s)}) y_-]\}^{-1} + \mathcal{O}(\bar{a}_0^6) = 0, \quad (\text{B1})$$

$$\left. \frac{\partial \mathcal{A}_{\bar{S}}^{[2/2]}}{\partial (\delta c_2)} \right|_{c_2^{(s)}} \equiv -\bar{a}_0^5 \{27(\delta c_2)^4 - 315c_1(\delta c_2)^3 y_- + 64z_0^4(c_2^{(s)}) y_-^2 [7c_1^2 - 2c_2^{(s)} + 3z_0^2(c_2^{(s)})] - 80c_1 \delta c_2 y_- \times [-2c_2^{(s)} y_-^2 - 2c_2^{(s)} z_0^2(c_2^{(s)}) + 12z_0^2(c_2^{(s)}) y_-^2 + 3z_0^4(c_2^{(s)}) + 7c_1^2(y_-^2 + z_0^2(c_2^{(s)}))] + 12(\delta c_2)^2 [-2c_2^{(s)} y_-^2 - 2c_2^{(s)} z_0^2(c_2^{(s)}) + 15z_0^2(c_2^{(s)}) y_-^2 + 3z_0^4(c_2^{(s)}) + c_1^2(82y_-^2 + 7z_0^2(c_2^{(s)}))] \} \times \{12y_-^4 [5c_1 \delta c_2 + 16y_-^3 - 8z_0^2(c_2^{(s)}) y_-]\}^{-1} + \mathcal{O}(\bar{a}_0^6) = 0. \quad (\text{B2})$$

The actual PMS-type equations are now obtained by requiring that the coefficients at $\sim \bar{a}_0^5$ in Eqs. (B1),(B2) be zero. When we have several possible solutions of the coupled system (26) and Eqs. (B1),(B2) for the three unknowns y_- , $c_2^{(s)}$, and δc_2 , we have to choose, in the PMS spirit, among the resulting approximants that one which has the smallest curvature. The curvature can be calculated by first obtaining the eigenvalues CA_1 and CA_2 of the curvature matrix C_A :

$$C_A = \begin{bmatrix} \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (c_2^{(1)})^2} & \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial c_2^{(1)} \partial c_2^{(2)}} \\ \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial c_2^{(1)} \partial c_2^{(2)}} & \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (c_2^{(2)})^2} \end{bmatrix}, \quad (\text{B3})$$

$$\begin{pmatrix} CA_1 \\ CA_2 \end{pmatrix} = \frac{1}{4} \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (c_2^{(s)})^2} + \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (\delta c_2)^2} \pm \left\{ \left(\frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (\delta c_2) \partial c_2^{(s)}} \right)^2 + \left[\frac{1}{4} \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (c_2^{(s)})^2} - \frac{\partial^2 \mathcal{A}_{\bar{S}}}{\partial (\delta c_2)^2} \right]^2 \right\}^{1/2}. \quad (\text{B4})$$

In the last expression, we traded $c_2^{(1)}$ and $c_2^{(2)}$ for $c_2^{(s)} \equiv (c_2^{(1)} + c_2^{(2)})/2$ and $\delta c_2 \equiv (c_2^{(1)} - c_2^{(2)})$. The curvature \mathcal{C}_A of the solution $\mathcal{A}_{\bar{S}}^{[2/2]}$ can be defined in at least two obvious ways which are virtually equivalent

$$\mathcal{C}_A = |CA_1| + |CA_2| \quad \text{or} \quad \mathcal{C}_A = \sqrt{(CA_1)^2 + (CA_2)^2}. \quad (\text{B5})$$

APPENDIX C: ECH AND TPS-PMS METHODS FOR NNLO TPS

The effective charge method (ECH) [3] of resummation of the NNLO TPS $S_{[2]}$ (2) can be expressed by employment of the subtracted version (A2) of Stevenson equation

$$\begin{aligned} & -r_1 + \frac{1}{a_0} + c_1 \ln \left(\frac{c_1 a_0}{1 + c_1 a_0} \right) \\ & + \int_0^{a_0} dx \frac{(c_2^{(0)} + c_3^{(0)} x + \dots)}{(1 + c_1 x)(1 + c_1 x + c_2^{(0)} x^2 + c_3^{(0)} x^3 + \dots)} \\ & = \frac{1}{a_{\text{ECH}}} + c_1 \ln \left(\frac{c_1 a_{\text{ECH}}}{1 + c_1 a_{\text{ECH}}} \right) \\ & + \int_0^{a_{\text{ECH}}} dx \frac{(\rho_2 + c_3 x + \dots)}{(1 + c_1 x)(1 + c_1 x + \rho_2 x^2 + c_3 x^3 + \dots)}. \end{aligned} \quad (\text{C1})$$

The ECH resummation value is $S^{\text{ECH}} = a_{\text{ECH}}$. In Eq. (C1), superscript “(0)” denotes the original RSch of $S_{[2]}$ (for example $\overline{\text{MS}}$ RSch with $n_f = 3$ in the considered BjPSR case), and c_3 denotes the NNLO ECH value of c_3 (in principle unknown at NNLO). Further, $c_2^{\text{ECH}} = \rho_2$, the latter RScl and RSch invariant is defined in Eq. (24). The coupling $a_0 \equiv \alpha_s^{(0)}/\pi$ is defined $a_0 \equiv a(\ln Q_0^2; c_2^{(0)}, c_3^{(0)}, \dots)$ as in Eq. (4), Q_0^2 being the original RScl in the TPS (chosen equal 3 GeV² in the considered BPSR case); $r_1 = -\beta_0 \ln(Q_{\text{ECH}}^2/Q_0^2)$ is the NLO TPS coefficient as staying in Eq. (2) at the original RScl Q_0^2 . In the above relation (C1), we often ignore the terms $\propto c_k^{(0)}$ and c_k ($k \geq 4$) since they are not known, i.e., we often choose the TPS form for the $\beta(x)$ functions. For a given value of a_0 , solving the above relation numerically for a_{ECH} gives us the resummed prediction for observable S . It is dependent on c_3 which, at this stage, is not known. More explicitly

$$S^{\text{ECH}}(c_3) = a_{\text{ECH}}(c_3) = a(\ln Q_{\text{ECH}}^2; \rho_2, c_3, \dots),$$

$$\text{with } Q_{\text{ECH}}^2 = Q_0^2 \exp(-r_1/\beta_0). \quad (\text{C2})$$

For the TPS-PMS method [2] applied to the NNLO TPS $S_{[2]}$, relation (C1) still remains valid, but with the replacements

$$a_{\text{ECH}}(c_3) \mapsto a_{\text{PMS}}(c_3), \quad c_2^{\text{ECH}} \equiv \rho_2 \mapsto c_2^{\text{PMS}} \equiv \frac{3}{2} \rho_2. \quad (\text{C3})$$

The resummed expression in the (NNLO) TPS-PMS case is the following TPS:

$$S^{\text{PMS}}(c_3) = a_{\text{PMS}} - \frac{1}{2} \rho_2 a_{\text{PMS}}^3, \quad \text{with}$$

$$a_{\text{PMS}}(c_3) = a(\ln Q_{\text{ECH}}^2; (3/2)\rho_2, c_3, \dots), \quad (\text{C4})$$

which again depends on c_3 . Expression (C4) is obtained by imposing PMS conditions on the TPS $S_{[2]}(\ln Q^2; c_2, c_3, \dots) = S^{\text{PMS}}$: $\partial S_{[2]} / \partial \ln Q^2 \sim a^5 \sim \partial S_{[2]} / \partial c_2$. It is straightforward to verify that, if $\rho_2 > 0$ (as in the considered BPSR case), S^{PMS} is bounded from above due to its specific TPS form: $S^{\text{PMS}} \leq (2/3)^{3/2} \rho_2^{-1/2}$, which in the considered BPSR case (36) is 0.2326 (because $\rho_2 = 5.476$).

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