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FROM THE NNLO QCD ANALYSIS
OF THE CCFR DATA
FOR THE xF_3 STRUCTURE FUNCTION

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Abstract

The more detailed next-to-next-to-leading order (NNLO) QCD analysis of the experimental data of the CCFR collaboration for the xF_3 structure function is performed. The factorization scale uncertainties are analyzed. The theoretical ambiguities of the results of our NNLO fits are estimated by means of the Padé resummation technique. The NNLO and the N³LO $\alpha_s(Q^2)$ \overline{MS} -matching conditions are used. In the process of the fits we are taking into account the twist-4 $1/Q^2$ -terms. We found that the amplitude of the x -shape of the twist-4 factor is consequently decreasing at the NLO and NNLO, though some remaining twist-4 structure seems to retain at the NNLO in the case when only statistical uncertainties are taken into account. The question of the stability of these results to the application of the [0/2] Padé resummation technique is considered. Our NNLO results for $\alpha_s(M_Z)$ values, extracted from the CCFR xF_3 data, are $\alpha_s(M_Z) = 0.118 \pm 0.002(stat) \pm 0.005(syst) \pm 0.003(theory)$ provided the twist-4 contributions are fixed through the infrared renormalon model and $\alpha_s(M_Z) = 0.121^{+0.007}_{-0.010}(stat) \pm 0.005(syst) \pm 0.003(theory)$ provided the twist-4 terms are considered as the free parameters.

1. Introduction.

Deep-inelastic lepton-nucleon scattering (DIS) belongs to the classical and continuously studying processes in modern particle physics. The traditionally measurable characteristics of νN DIS are the SFs F_2 and xF_3 . It should be stressed that the program of getting information about the behavior of the SFs of νN DIS is among the aims of the experimental program of Fermilab Tevatron and CCFR/NuTeV collaboration in particular. The CCFRR collaboration started to study the νN scattering process in 1980 [1]. The data for the SFs of νN DIS, obtained by the follower of the CCFRR collaboration, namely the CCFR group, was distributed among the potential users in the beginning of 1997 [2], while the final results of the original CCFR DGLAP [3] NLO analysis of this data was presented in the journal publication of Ref.[2].

This experimental information was already used in the process of different NLO analysis, performed by CTEQ, MRST and GRV groups (see Refs.[4, 5, 6] correspondingly). The subsequent steps of performing NLO and the first NNLO analysis of the CCFR data with the help of the Jacobi polynomial - Mellin moments version of the DGLAP method were made in Refs.[7]-[12] (the definite stages in the development of this formalism are described in Refs.[13]-[15]).

In the process of the analysis of Refs.[9]-[12] the authors used important information about the NNLO corrections to the coefficient functions [16] and results of the complicated analytical calculations of the NNLO corrections to the anomalous dimensions of the NS moments with $n = 2, 4, 6, 8, 10$ [17], supplemented with the estimated values of the NNLO coefficients of the anomalous dimensions of $n = 3, 5, 7, 9$ NS moments, which were obtained in Ref.[9] with the help of the smooth interpolation procedure, previously proposed in Ref.[18]. Moreover, the attempts to extract the shape of the twist-4 contributions and study the predictive abilities of the IR-renormalon (IRR) model of Ref.[19] were made (for the definite details of modeling the effects of the power-suppressed contributions to xF_3 and other measurable physical quantities within the IRR language see Ref.[20] and Ref.[21] correspondingly, for more details see the review of Ref.[22]).

However, the important question of estimating theoretical uncertainties of the NNLO analysis of the CCFR data of Ref.[11] was still non-analyzed in detail. These uncertainties can be specified in part after taking into account

- 1) the differences in the definitions of $\alpha_s(Q^2)$ matching conditions (see e.g. Refs.[23, 24, 25, 26]), which are responsible for penetrating into the energy region, characteristic for the $f = 5$ numbers of flavours, where the pole of the Z^0 -boson is manifesting itself;

- 2) corrected in Ref.[27] NNLO QCD contribution to the matching condition of Ref.[23] and the 4-loop coefficient of the QCD β -function [28], which is entering into the N³LO approximation of the renormalization group evolution equation for the Mellin moments, the N³LO expression for the coupling constant and in the calculated N³LO-term [29] in the matching condition of Ref.[23];

- 3) the theoretical uncertainties due to non-calculated N³LO contributions into the coefficient functions and the anomalous dimensions functions;

- 4) at the NNLO it is also desirable to analyse carefully the dependence of the results obtained from the choice of the Jacobi polynoms parameters α and β (see definitions beyond), which are entering into the theoretical expression for the reconstructed structure function (at the NLO this problem was studied in detail in Ref.[15]). This analysis is of relevant importance in view of the appearance of the doubts in the applicability of the Jacobi evolution method (see Ref.[30]), which, however, were immediately dispelled in Ref.[31];

- 5) last, but not least, uncertainties are related to the problems of factorization and renormalization scales choice. It is worth to note that these problems are in relation with fixing the ambiguities due to already calculated and uncalculated N³LO QCD effects, which can be modeled using the Padé resummation technique.

This work is devoted to the analysis of the important problems outlined above and to the

more detailed extraction of the values of $\alpha_s(M_Z)$ and the x -shape of the twist-4 power-suppressed term at available orders of perturbative QCD taking into account the effects enumerated above. We are supplementing the NNLO fits of Ref.[11] by the N³LO analysis, which is based on the application of the Padé resummation technique (for a review see Ref.[32]), developed in QCD in the definite form in Refs.[33, 34] and considered previously as the possible method of fixing theoretical uncertainties in the analysis of DIS data in Ref.[35]. It should be stressed that *a posteriori* this technique gives results similar to those obtained with the help of different methods of fixing scale-scheme dependence ambiguities (compare the results of Ref.[36] with the results of Refs.[33, 34] obtained using the Padé resummation technique). Thus, our analysis could be considered as the attempt to estimate perturbative QCD uncertainties beyond the NNLO level. Moreover, it could give us the hint whether the outcomes of the NNLO fits, related to perturbative and non-perturbative sectors, stay stable after the inclusion of the explicitly calculated and estimated N³LO QCD corrections.

Another new important ingredient of our analysis, discussed in brief in Ref.[37], is the analysis of the problem of the factorization scale choice. In particular, we will demonstrate that due to the unnaturally large NNLO corrections to the renormalization-group improved $n=2$ Mellin moment of the xF_3 SF, it is essential to choose the value of the factorization point in the vicinity of the scale $Q_0^2=20 \text{ GeV}^2$.

2. The theoretical background of the QCD analysis.

Let us define the Mellin moments for the NS SF $xF_3(x, Q^2)$:

$$M_n^{NS}(Q^2) = \int_0^1 x^{n-1} F_3(x, Q^2) dx \quad (1)$$

where $n = 2, 3, 4, \dots$. The theoretical expression for these moments obey the following renormalization group equation

$$\left(\mu \frac{\partial}{\partial \mu} + \beta(A_s) \frac{\partial}{\partial A_s} + \gamma_{NS}^{(n)}(A_s) \right) M_n^{NS}(Q^2/\mu^2, A_s(\mu^2)) = 0 \quad (2)$$

where $A_s = \alpha_s/(4\pi)$. The renormalization group functions are defined as

$$\begin{aligned} \mu \frac{\partial A_s}{\partial \mu} = \beta(A_s) &= -2 \sum_{i \geq 0} \beta_i A_s^{i+2} \\ \mu \frac{\partial \ln Z_n^{NS}}{\partial \mu} = \gamma_{NS}^{(n)}(A_s) &= \sum_{i \geq 0} \gamma_{NS}^{(i)}(n) A_s^{i+1} \end{aligned} \quad (3)$$

where Z_n^{NS} are the renormalization constants of the corresponding NS operators. The solution of the renormalization group equation can be presented in the following form :

$$\frac{M_n^{NS}(Q^2)}{M_n^{NS}(Q_0^2)} = \exp \left[- \int_{A_s(Q_0^2)}^{A_s(Q^2)} \frac{\gamma_{NS}^{(n)}(x)}{\beta(x)} dx \right] \frac{C_{NS}^{(n)}(A_s(Q^2))}{C_{NS}^{(n)}(A_s(Q_0^2))} \quad (4)$$

where $M_n^{NS}(Q_0^2)$ is the phenomenological quantity related to the factorization scale dependent factor. At fixed momentum transfer Q_0^2 it will be parameterized in the simple form

$$M_n^{NS}(Q_0^2) = \int_0^1 x^{n-2} A(Q_0^2) x^{b(Q_0^2)} (1-x)^{c(Q_0^2)} (1+\gamma(Q_0^2)x) dx \quad (5)$$

with $\gamma \neq 0$ or $\gamma = 0$. It is identical to the form used by the CCFR collaboration [2]. In principle, following the models of parton distributions used in Refs.[5, 6], one can add in Eq.(5) the term, proportional to \sqrt{x} . However, since this term is only important in the region of rather small x , we will neglect it in our analysis.

At the N^3LO the expression for the coefficient function $C_{NS}^{(n)}$ can be defined as

$$C_{NS}^{(n)}(A_s) = 1 + C^{(1)}(n)A_s + C^{(2)}(n)A_s^2 + C^{(3)}(n)A_s^3, \quad (6)$$

while the corresponding expansion of the anomalous dimensions term is

$$\exp\left[-\int^{A_s(Q^2)} \frac{\gamma_{NS}^{(n)}(x)}{\beta(x)} dx\right] = (A_s(Q^2))^{\gamma_{NS}^{(0)}(n)/2\beta_0} \times AD(n, A_s) \quad (7)$$

where

$$AD(n, A_s) = [1 + p(n)A_s(Q^2) + q(n)A_s(Q^2)^2 + r(n)A_s(Q^2)^3] \quad (8)$$

and $p(n)$, $q(n)$ and $r(n)$ have the following form:

$$p(n) = \frac{1}{2} \left(\frac{\gamma_{NS}^{(1)}(n)}{\beta_1} - \frac{\gamma_{NS}^{(0)}(n)}{\beta_0} \right) \frac{\beta_1}{\beta_0} \quad (9)$$

$$q(n) = \frac{1}{4} \left(2p(n)^2 + \frac{\gamma_{NS}^{(2)}(n)}{\beta_0} + \gamma_{NS}^{(0)}(n) \frac{(\beta_1^2 - \beta_2\beta_0)}{\beta_0^3} - \gamma_{NS}^{(1)}(n) \frac{\beta_1}{\beta_0^2} \right) \quad (10)$$

$$r(n) = \frac{1}{6} \left(p(n)^3 + 6p(n)q(n) + \frac{\gamma_{NS}^{(3)}(n)}{\beta_0} - \frac{\beta_1\gamma_{NS}^{(2)}(n)}{\beta_0^2} - \frac{\beta_2\gamma_{NS}^{(1)}(n)}{\beta_0^2} + \frac{\beta_1^2\gamma_{NS}^{(1)}(n)}{\beta_0^3} - \frac{\beta_1^3\gamma_{NS}^{(0)}(n)}{\beta_0^4} - \frac{\beta_3\gamma_{NS}^{(0)}(n)}{\beta_0^2} + \frac{2\beta_1\beta_2\gamma_{NS}^{(0)}(n)}{\beta_0^3} \right) \quad (11)$$

The coupling constant $A_s(Q^2)$ can be expressed in terms of the inverse powers of $L = \ln(Q^2/\Lambda_{MS}^2)$ as $A_s^{NLO} = A_s^{LO} + \Delta A_s^{NLO}$, $A_s^{NNLO} = A_s^{NLO} + \Delta A_s^{NNLO}$ and $A_s^{N^3LO} = A_s^{NNLO} + \Delta A_s^{N^3LO}$, where

$$A_s^{LO} = \frac{1}{\beta_0 L} \quad (12)$$

$$\Delta A_s^{NLO} = -\frac{\beta_1 \ln(L)}{\beta_0^3 L^2}$$

$$\Delta A_s^{NNLO} = \frac{1}{\beta_0^5 L^3} [\beta_1^2 \ln^2(L) - \beta_1^2 \ln(L) + \beta_2\beta_0 - \beta_1^2] \quad (13)$$

$$\Delta A_s^{N^3LO} = \frac{1}{\beta_0^7 L^4} [\beta_1^3 (-\ln^3(L) + \frac{5}{2} \ln^2(L) + 2 \ln(L) - \frac{1}{2}) - 3\beta_0\beta_1\beta_2 \ln(L) + \beta_0^2 \frac{\beta_3}{2}] \quad (14)$$

Notice that in our normalization the numerical expressions for β_0 , β_1 , β_2 and β_3 read

$$\begin{aligned} \beta_0 &= 11 - 0.6667f \\ \beta_1 &= 102 - 12.6667f \\ \beta_2 &= 1428.50 - 279.611f + 6.01852f^2 \\ \beta_3 &= 29243.0 - 6946.30f + 405.089f^2 + 1.49931f^3 \end{aligned} \quad (15)$$

where the expression for β_3 was obtained in Ref.[28]. The inverse-log expansion for $\Delta A_s^{N^3LO}$, which incorporates the information about the coefficient β_3 , was presented in Ref.[29].

Few words ought to be said about the used approximation for the anomalous dimension function $\gamma_{NS}^{(n)}(A_s)$. The analytical expression for its one-loop coefficient is well-known: $\gamma_{NS}^{(0)}(n) = (8/3)[4\sum_{j=1}^n (1/j) - 2/n(n+1) - 3]$. In the cases of both F_2 and xF_3 SFs the numerical expressions for $\gamma_{NS}^{(1)}(n)$ -coefficients are given in Table 1.

n	$\gamma_{NS,F_2}^{(1)}(n)$	$\gamma_{NS,F_3}^{(1)}(n)$	$\gamma_{NS}^{(2)}(n)$	$\gamma_{NS}^{(3)}(n) _{[1/1]}$	$\gamma_{NS}^{(3)}(n) _{[0/2]}$
2	71.374	71.241	612.1	5259	5114
3	100.801	100.782	837.4	6959	6900
4	120.145	120.140	1005.8	8421	8414
5	134.905	134.903	1135.8	9563	9562
6	147.003	147.002	1242.0	10493	10482
7	157.332	157.332	1334.0	11310	11280
8	166.386	166.386	1417.5	12077	12012
9	174.468	174.468	1493.5	12784	12706
10	181.781	181.781	1559.0	13370	13271
11	188.466	188.466	?	?	?
12	194.629	194.629	?	?	?
13	200.350	200.350	?	?	?
14	205.689	205.689	?	?	?

Table 1. The used numerical expressions for the NLO and NNLO coefficients of the anomalous dimensions of the moments of the NS SFs at $f = 4$ number of flavours and the N³LO Padé estimates.

These results are normalized to the world with $f = 4$ numbers of active flavours. In the same Table we present the numerical expressions for $\gamma_{NS}^{(2)}(n)$, used in the process of the fits. In the cases of $n = 2, 4, 6, 8, 10$ they follow from the explicit calculations of $\gamma_{NS,F_2}^{(2)}(n)$ -terms [17], normalized to $f = 4$, while the $n = 3, 5, 7, 9$ numbers were fixed using the smooth interpolation procedure, originally proposed in Ref.[18]. Note in advance, that since $\gamma_{NS,F_3}^{(2)}(n)$ -coefficients differ from $\gamma_{NS,F_2}^{(2)}(n)$ -terms, though by the presumably small additional contributions (for discussions see Ref.[9]), it would be interesting to verify the precision of the expression for $\gamma_{NS}^{(2)}(n)$, used in the process of our NNLO xF_3 fits, by the explicit analytical calculations of the NNLO contributions to the anomalous dimensions of odd moments of the xF_3 structure function.

Let us now describe the procedure of fixing other theoretical uncertainties. After the work of Ref.[33] it became rather popular to model the effects of the higher order terms of perturbative series in QCD using the expanded Padé approximants.

In the framework of this technique the values of the terms $C^{(3)}(n)$ and $r(n)$ could be expressed as

$$Padé [1/1] : \quad C^{(3)}(n) = [C^{(2)}(n)]^2 / C^{(1)}(n) \quad (16)$$

$$r(n) = q(n)^2 / p(n) \quad (17)$$

$$Padé [0/2] : \quad C^{(3)}(n) = 2C^{(1)}(n)C^{(2)}(n) - [C^{(1)}(n)]^3 \quad (18)$$

$$r(n) = 2p(n)q(n) - [p(n)]^3 \quad (19)$$

The numerical values for $p(n)$ and $q(n)$, obtained from the results of Table 1 and definitions of Eqs.(9)-(11), together with the values of the coefficients $C^{(1)}(n)$ and $C^{(2)}(n)$ (which come from the calculations of Ref.[16]), are presented in Table 2.

n	$p(n)$	$q(n)$	$r(n) _{[1/1]}$	$r(n) _{[0/2]}$	$C^{(1)}(n)$	$C^{(2)}(n)$	$C^{(3)}(n) _{[1/1]}$	$C^{(3)}(n) _{[0/2]}$
2	1.646	4.232	10.829	9.476	-1.778	-47.472	-1268	174
3	1.941	4.774	11.738	11.218	1.667	-12.715	97	-47
4	2.050	5.546	15.003	14.123	4.867	37.117	283	246
5	2.115	6.134	17.790	16.486	7.748	95.408	1175	1013
6	2.165	6.595	20.087	18.407	10.351	158.291	2421	2168
7	2.210	7.039	22.421	20.318	12.722	223.898	3940	3638
8	2.252	7.525	25.138	22.471	14.900	290.884	5679	5360
9	2.294	8.018	28.027	24.715	16.915	358.587	7602	7291
10	2.334	8.375	30.049	26.382	18.791	426.442	9677	9391

Table 2. The values for the NLO and NNLO QCD contributions used in our fits and the N³LO Padé estimates.

In the same Table we also give the estimates for $r(n)$ and $C^{(3)}(n)$, obtained using the expanded [1/1] and [0/2] Padé approximants formulae of Eqs.(16)-(19). For the sake of completeness in the last two columns of Table 1 we also present the estimates for the N³LO contributions to the anomalous dimension function $\gamma_{NS}^{(n)}(A_s)$, obtained with the help of the expanded [1/1] and [0/2] Padé approximants. One can see that the results of applications of [1/1] and [0/2] Padé approximants for $\gamma_{NS}^{(3)}(n)$ are almost identical to each other.

Using the numbers presented in Table 1, one can construct Padé motivated expressions for $r(n)$ by substituting the estimates for $\gamma_{NS}^{(3)}(n)$ into Eq.(11). It should be stressed, that obtained in this way, estimates for $r(n)$ will qualitatively agree with the ones presented in Table 2 within the “Padé world” only, namely only in the case of application in Eq.(11) of the [1/1] or [0/2] Padé estimate for the four-loop coefficient of the QCD β -function β_3 . However, in the case of $f = 4$ the direct application of the [1/1] and [0/2] Padé approximants underestimates the calculated value of β_3 by the factor of over 2.5 ($\beta_3|_{[1/1]} \approx 3217$; $\beta_3|_{[0/2]} \approx 3058$). In view of this, the application of Eq.(11) with the Padé estimated values of $\gamma_{NS}^{(3)}(n)$ and the explicit expression for β_3 -coefficient are giving estimates of $r(n)$, drastically different from the ones presented in Table 2 (for example, for the case of application of [0/2] Padé estimates it gives $r(2) \approx 18.83, \dots, r(10) \approx 55.70$).

It is already known that the accuracy of the estimates of the N³LO coefficient of the QCD β -function can be improved by some additional fits of polynomial dependence of β_3 from the number of flavours f and applying the asymptotic Padé approximant (APAP) formula [38]. Therefore, it might be interesting to think about the possibility of putting bold guess Padé estimates of N³LO contributions to $\gamma_{NS}(A_s)$ (see Table 1) on a more solid background. The analogous steps were already done in Ref.[39] in the case of the analysis of the status of N³LO Padé estimates for the anomalous dimension function of quark mass. The agreement of the obtained estimates with the calculated four-loop QCD results of Ref.[40, 41] turned out to be reasonable. One can hope, that the application of the similar procedure for the APAP estimates of $\gamma_{NS}^{(3)}$ -terms and the substitution of the results obtained in Eq.(11) (together with the explicit expression for the β_3 -term) might improve the agreement with the estimates, presented in Table 2, which at this step we consider as the most suitable results for modeling the unknown effects of the N³LO corrections, which depend from the N³LO expression for the coupling constant A_s .

Within this approach the uncertainties of the results of the NNLO fits can be estimated by modeling $q(n)$ and $C^{(2)}(n)$ using the [0/1] Padé approximants, which give $q(n)|_{[0/1]} = [p(n)]^2$ and $C^{(2)}(n)|_{[0/1]} = [C^{(1)}(n)]^2$. The estimated values of $q(n)|_{[0/1]}$ have the correct sign for $n \geq 2$, while for $C^{(2)}(n)$ the same feature takes place in the case of $n \geq 4$ moments. Moreover, for $n \geq 4$ the relative values of the ratios $q(n)|_{[0/1]}/q(n)$ are varying from 1.3 to 1.5, while the similar ratios for the NLO contributions to the coefficient function $C^{(2)}(n)|_{[0/1]}/C^{(2)}(n)$ are changing from 1.6

at $n = 4$ to 1.2 at $n = 10$. This precision seems to be rather acceptable for the $[0/1]$ Padé estimates, which in the case of each concrete fixed value of n are based on one input term of the corresponding perturbative series.

It should also be stressed that the uncertainties of the values of $r(n)$ are not so important, since the results of our fits will be more sensitive to the form of the Padé approximations predictions for the N³LO contributions into the coefficient function (namely $C^{(3)}(n)$ -terms).

From the results presented in Table 2 one can conclude, that the theoretical series for $C_{NS}^{(n)}$ for large n ($n \geq 4$), which are relevant to the behavior of $x F_3(x, Q^2)$ SF in the intermediate and large x -region, probably have sign nonalternating structure with asymptotically increasing positive coefficients. Therefore, the applications of the expanded $[1/1]$ and $[0/2]$ Padé approximants for estimating the terms $C^{(3)}(n)$ with $n \geq 4$ (which in both cases have the same positive sign and the same order of magnitude) might be considered as the useful ingredient for the N³LO Padé-motivated fits.

However, in the cases of the coefficient functions of $n = 2, 3$ moments of the $x F_3$ SF our intuition does not give us the idea what might be the sign and order of magnitude of the third term in perturbative series $C_{NS}^{(2)}(A_s) = 1 - 1.78 A_s - 47.47 A_s^2$ and $C_{NS}^{(3)}(A_s) = 1 + 1.67 A_s - 12.71 A_s^2$. Indeed, in these two cases the manipulations with $[1/1]$ and $[0/2]$ Padé approximants are giving drastically different estimates for the terms $C^{(3)}(n)$, which in the cases of $n = 2, 3$ differ both by sign and size (see Table 2). It is possible that this feature is related to the fact that for $n = 2, 3$ the coefficients of $C_{NS}^{(n)}(A_s)$ do not have the immediate $(+1)^n n!$ growth, but poses some zigzag structure, which is manifesting itself in the cases of definite perturbative series of quantum field theory models (for discussions see e.g. Ref.[42]). This might give the additional theoretical uncertainties of modeling higher-order perturbative QCD predictions for $x F_3(x, Q^2)$ in the region of relatively small x .

In view of the questionable asymptotic behavior of the NNLO series for the coefficient functions of the NS moments with low n ($n = 2, 3$) we are also using the idea of Ref.[35] and consider the results of applications of non-expanded Padé approximants in the process of the analysis of the DIS data.

Let us recall that the corresponding non-expanded $[1/1]$ Padé approximants can be defined as

$$AD(n, A_s)|_{[1/1]} = \frac{1 + a_1^{(n)} A_s}{1 + b_1^{(n)} A_s} \quad (20)$$

$$C_{NS}^{(n)}(A_s)|_{[1/1]} = \frac{1 + c_1^{(n)} A_s}{1 + d_1^{(n)} A_s} \quad (21)$$

where $a_1^{(n)} = \left([p(n)]^2 - q(n) \right) / p(n)$, $b_1^{(n)} = -q(n) / p(n)$ and $C_1^{(n)} = \left([C^{(1)}(n)]^2 - C^{(2)}(n) \right) / C^{(1)}(n)$, $d_1^{(n)} = -C^{(2)}(n) / C^{(1)}(n)$.

The explicit expressions for the non-expanded $[0/2]$ Padé approximants read:

$$AD(n, A_s)|_{[0/2]} = \frac{1}{1 + b_1^{(n)} A_s + b_2^{(n)} A_s^2} \quad (22)$$

$$C_{NS}^{(n)}(A_s)|_{[0/2]} = \frac{1}{1 + d_1^{(n)} A_s + d_2^{(n)} A_s^2} \quad (23)$$

where $b_1^{(n)} = -p(n)$, $b_2^{(n)} = p(n)^2 - q(n)$, $d_1^{(n)} = -C^{(1)}(n)$ and $d_2^{(n)} = [C^{(1)}(n)]^2 - C^{(2)}(n)$. Since we consider the applications of both $[1/1]$ and $[0/2]$ Padé approximants as attempts to model the behavior of the perturbative series for the NS Mellin moments beyond the NNLO level, we will use in Eqs.(20)-(23) the N³LO expression for the coupling constant A_s , defined

through Eqs.(12)-(14). It is worth to mention here, that quite recently the expanded and non-expanded Padé approximants were successfully used for the study of the N³LO approximation of the ground state energy in quantum mechanics [43] and of the behavior of the β -function for the quartic Higgs coupling in the Standard Electroweak Model [44].

The next step is the reconstruction of the structure function $xF_3(x, Q^2)$ with both target mass corrections and twist-4 terms taken into account. The reconstructed SF can be expressed as:

$$xF_3^{N_{max}}(x, Q^2) = w(\alpha, \beta)(x) \sum_{n=0}^{N_{max}} \Theta_n^{\alpha, \beta}(x) \sum_{j=0}^n c_j^{(n)}(\alpha, \beta) M_{j+2, xF_3}(Q^2) + \frac{h(x)}{Q^2} \quad (24)$$

where $\Theta_n^{\alpha, \beta}$ are the Jacobi polynomials, α, β are their parameters, fixed by the condition of the requirement of the minimization of the error of the reconstruction of the SF, and $w(\alpha, \beta) = x^\alpha(1-x)^\beta$ is the corresponding weight function. In order to take into account the target mass corrections the Nachtmann moments

$$M_{n, xF_3} \rightarrow M_{n, xF_3}^{TMC}(Q^2) = \int_0^1 \frac{dx \xi^{n+1}}{x^2} F_3(x, Q^2) \frac{1 + (n+1)V}{(n+2)}, \quad (25)$$

can be used, where $\xi = 2x/(1+V)$, $V = \sqrt{1 + 4M_{nucl}^2 x^2/Q^2}$ and M_{nucl} is the mass of a nucleon. However, to simplify the analysis it is convenient to expand equation (25) into a series in powers of M_{nucl}^2/Q^2 [45]. Taking into account the order $O(M_{nucl}^4/Q^4)$ corrections, we get

$$M_{n, xF_3}^{TMC}(Q^2) = M_{n, xF_3}^{NS}(Q^2) + \frac{n(n+1)}{n+2} \frac{M_{nucl}^2}{Q^2} M_{n+2, xF_3}^{NS}(Q^2) + \frac{(n+2)(n+1)n}{2(n+4)} \frac{M_{nucl}^4}{Q^4} M_{n+4, xF_3}^{NS}(Q^2) + O\left(\frac{M_{nucl}^6}{Q^6}\right), \quad (26)$$

We have checked that the order $O(M_{nucl}^4/Q^4)$ terms in Eq.(26) have a rather small effect in the process of the concrete fits. Therefore, in what follows we will use only the first two terms in the r.h.s. of Eq.(26).

The form of the twist-4 contributions $h(x)$ in Eq.(24) was first fixed as

$$\frac{h(x)}{Q^2} = w(\alpha, \beta) \sum_{n=0}^{N_{max}} \Theta_n^{\alpha, \beta}(x) \sum_{j=0}^n c_j^{(n)}(\alpha, \beta) M_{j+2, xF_3}^{IRR}(Q^2) \quad (27)$$

where $c_j^{(n)}(\alpha, \beta)$ are the polynomials, which contain α and β -dependent Euler Γ -functions and

$$M_{n, xF_3}^{IRR}(Q^2) = \tilde{C}(n) M_{n, xF_3}^{NS}(Q^2) \frac{A'_2}{Q^2} + O\left(\frac{1}{Q^4}\right) \quad (28)$$

with A'_2 taken as the free parameter and $\tilde{C}(n)$ defined following the IRR model estimates of Ref.[19] as $\tilde{C}(n) = -n - 4 + 2/(n+1) + 4/(n+2) + 4S_1(n)$ ($S_1(n) = \sum_{j=1}^n 1/j$). It should be stressed that the appearance of the multiplicative QCD expression $M_{n, xF_3}^{NS}(Q^2)$ in Eq.(28), generally speaking different from the intrinsic coefficient function of the twist-4 contribution, is leading to theoretical uncertainties in the contributions of higher-order QCD corrections to the twist-4 part of the $xF_3(x, Q^2)$ SF. This could provide the additional theoretical errors in

the studies of the status of the IRR-model predictions for the twist-4 terms at the NNLO and beyond.

In order to analyse this question at a more definite theoretical level it is instructive to model the function $h(x)$ by the additional free parameters of the fits, not related to the IRR-model predictions.

We will estimate the uncertainties of the values of $\Lambda_{\overline{MS}}^{(4)}$, and thus $\alpha_s(M_Z)$, by studying the factorization scale dependence of the outcomes of the fits. We will also analyse the stability of the extracted values of the IRR-model parameter A'_2 and the twist-4 function $h(x)$ to the inclusion of the explicitly calculated N³LO QCD corrections and other unknown N³LO terms (modeled with the help of the Padé resummation technique) into the fits of the concrete data. Our aim will also be the study of the influence of the choice of the initial factorization scale to the results of Ref.[11] and especially to the ones, which are describing the x -shape of $h(x)$ for the xF_3 SF within the method adopted by us.

3 (a). The analysis of the experimental data: the extraction of $\Lambda_{\overline{MS}}^{(4)}$ vs α_s value.

The results for our NLO and NNLO fits, made for the case of $f = 4$ number of active flavours, are presented in Table 1 of Ref.[11], where the values of the parameters for the model of the xF_3 SF $A, b, c, \gamma \neq 0$ (which are related to the parton distribution parameters) are also given. The results of Ref.[11] were obtained using the fixed value of the factorization point $Q_0^2 = 5 \text{ GeV}^2$ and the fixed weight function of the Jacobi polynomials reconstruction formula of Eq.(24), namely $x^{0.7}(1-x)^3$, which is similar to the x -shape of the NS structure function itself and is in agreement with the quark-counting rules of Ref.[46] at large x and is close to the Redge theory behaviour of the NS SF at small x .

In this section we will present more definite arguments in favour of the used form of the Jacobi polynomials weight function and will study the factorization scale dependence of the results for $\Lambda_{\overline{MS}}^{(4)}$, extracted at different orders of perturbation theory.

We will also construct the N³LO Q^2 -evolution equations for the Mellin moments using the Padé approximants, written down both in the expanded and non-expanded forms. In the process of these “approximate” N³LO fits, the explicit N³LO expression for the QCD running coupling constant A_s , defined in Eqs.(12)-(15), will be used. Thus we obtain from the fits the N³LO estimates of the values of the parameter $\Lambda_{\overline{MS}}^{(4)}$ (and therefore $\alpha_s(M_Z)$), and of the common factor A'_2 of the IRR model. The comments on the attempts to apply the scheme-invariant analysis for estimating the renormalization-scheme dependence of the results obtained will also be presented.

It should be stressed that despite the general theoretical preference of applications of the diagonal Padé approximants (for the recent analysis see e.g. Ref.[47]), the N³LO [1/1] Padé approximant description of the CCFR'97 experimental data turned out to be not acceptable in our case, since it produces a rather high value of χ^2 : $\chi^2/nep > 2$ (where $nep = 86$ is the number of the experimental points, taken into account in the case of the cut $Q^2 > 5 \text{ GeV}^2$). However, the application of [0/2] Padé approximants produced reasonable results. We think that the non-applicability of the [1/1] Padé method in the process of fitting CCFR xF_3 data with the help of the Jacobi polynomials approach can be related to the manifestation of a rather large value of the ratio $[C^{(3)}(2)/C^{(2)}(2)]|_{[1/1]}$ in the expression for the NS moment M_{2,xF_3}^{NS} (see Table 2).

The similar effect of the preference of the [0/2] Padé approximant analysis over the [1/1] one was found in Ref.[34] in the case of the comparison of the QCD theoretical predictions for the polarized Bjorken sum rule (which are closely related to the QCD predictions for the first moment of the xF_3 SF, namely for the Gross-Llewellyn Smith sum rule) with the available experimental data.

Considering the problem of the minimization of the dependence of the results of the fits from

free parameters α, β to the way of fixing them we found several minimum on the (α, β) - plane at $Q_0^2 = 5 \text{ GeV}^2$:

1. Minimum A: $\alpha/\beta \approx -0.6/0.55$.

In this minimum we got the reasonable LO, NLO and NNLO values of $\Lambda_{\overline{MS}}^{(4)}$ for $N_{max} = 6$. However, the manifestation of this minimum strongly depends from the number of moments taken into account. For example, in the case of $N_{max} = 10$ we were unable to find this minimum at the LO and NLO, so we are considering this minimum as spurious one;

2. Minimum B : $\alpha/\beta \approx -0.5/-0.9$.

This minimum is appearing at the LO and NLO. However, this minimum is not appearing at the NNLO, so we consider it as the non-applicable for our NNLO fits.

3. Minimum C: $\alpha/\beta \approx 0.8/1.3$.

For $N_{max} = 6$ the LO and NLO values of $\Lambda_{\overline{MS}}^{(4)}$ can be obtained. However, at the NNLO this minimum does not manifest itself. Moreover, it is disappearing at the LO and NLO for the case of $N_{max} = 10$. Therefore, we are considering it as the spurious one also.

4. Minimum D: $\alpha/\beta \approx 0.6/-0.99$.

It should be stressed, that at the LO and NLO this minimum is appearing only for $N_{max} = 6$ and is disappearing for $N_{max} = 10$. Moreover, the obtained value of β is giving the unnatural singular $1/(1-x)$ behaviour of the Jacobi polynomial weight function $w(\alpha, \beta)$. In view of this we consider this minimum as the unphysical one.

5. Minimum E: $\alpha/\beta \sim 0.7/3.0$.

This is the minimum, in which we were working previously in Refs.[11, 12]. In this minimum the results of LO and NLO fits are in agreement with the ones obtained in Refs.[11, 12]. It should be noted that at the LO and NLO this minimum is stable due to variation of Q_0^2 and to the inclusion of the higher Mellin moments into the reconstruction formulae of Eq.(24) and Eq.(27) (we have checked this foundation, repeating the fits for $N_{max} = 10$). At the NNLO this minimum is appearing at Q_0^2 higher than 10 GeV^2 .

Since the values of the parameters α, β in the Minimum E are almost identical to the initially considered ones($\alpha = 0.7, \beta = 3$) and in view of the stability of the results of the LO and NLO fits to the value of the factorization point Q_0^2 , we consider this minimum as the physical one and will be working in its vicinity, fixing $\alpha = 0.7$ and $\beta = 3$ as previously.

In order to study the factorization scale dependence in more detail and thus to estimate the factorization scale uncertainties of the results, obtained in Refs.[11, 12], we performed LO, NLO and NNLO fits for different values of the factorization scale without taking into account twist-4 contributions, but with target mass corrections included (see Ref.[37]). The results for $\Lambda_{\overline{MS}}^{(4)}$ are presented in Table 3.

$Q_0^2 (\text{GeV}^2)$	5	8	10	20	50	100
LO	266±35	266±35	265±34	264±35	264±36	263±36
LO*	382±38	380±41	380±40	379±46	378±43	377±42
NLO	341±30	340±40	340±35	339±36	337±34	337±37
NLO*	322±29	321±33	321±33	320±34	319±36	318±36
NNLO	293±30	312±33	318±33	326±35	326±36	325±36
NNLO*	284±28	312±33	318±33	326±35	326±36	325±36
N ³ LO [0/2]	293±29	323±32	330±35	335±37	326±36	319±35

Table 3. The Q_0^2 dependence of $\Lambda_{\overline{MS}}^{(4)}$ [MeV]. The LO* means that in the LO-fits NLO α_s is used; NLO* (NNLO*) indicates that in the NLO (NNLO) fits NNLO (N³LO) α_s is used. N³LO [0/2] marks the results of the expanded [0/2] Padé fits with α_s defined at the N³LO.

One can see, that the LO and NLO results are stable to the variation of Q_0^2 . The results of LO* fits are higher than the LO ones, and from this level taking into account other perturbative QCD effects tend to decrease the values of $\Lambda_{\overline{MS}}^{(4)}$ up to the level of the NNLO*-fits.

The NNLO results are sensitive to the variation of the factorization scale Q_0^2 . The values of $\Lambda_{\overline{MS}}^{(4)}$ become stable for $Q_0^2 \geq 10 \text{ GeV}^2$ only. The same effect is manifesting itself for the results of the expanded [0/2] Padé approximants fits, which incorporate the explicit information about the N³LO expression for the coupling constant A_s . We think that this effect might be related to a rather peculiar behaviour of the NNLO perturbative QCD expression of $n = 2$ moment. Indeed, taking into account the exact numerical values of the coefficients $p(2)$, $q(2)$, $C^{(1)}(2)$ and $C^{(2)}(2)$ from Table 2, we find that the perturbative behaviour of this moment is determined by the following perturbative series

$$AD(2, A_s)C_{NS}^{(2)}(A_s) = 1 - 0.132A_s(Q^2) - 46.155A_s^2(Q^2) + \dots \quad (29)$$

where the relatively large A_s^2 coefficient is dominated by the NNLO term of the coefficient function of $n = 2$ moment. Thus we think that it is safer to start the QCD evolution from the factorization scale $Q_0^2 = 20 \text{ GeV}^2$, where the numerical value of the A_s^2 contribution in Eq.(29) is smaller. Note, that this choice of the factorization point is also empirically supported by the fact that it is lying in the mid of Q^2 kinematic region of the CCFR data.

In Table 4 we are presenting the results of our new fits for $\Lambda_{\overline{MS}}^{(4)}$ and IRR-model parameter A'_2 obtained at LO, NLO, NNLO and N³LO (modeled by the expanded and non-expanded Padé approximants) in the cases of both $\gamma \neq 0$ and $\gamma = 0$. The factorization point is fixed at $Q_0^2 = 20 \text{ GeV}^2$.

Looking carefully at Table 4 we arrive at the following conclusions:

- The results of LO and NLO fits are identical to the ones obtained in Ref.[11].
- Our fits demonstrate that the NNLO values of the parameter $\Lambda_{\overline{MS}}^{(4)}$ depend from the choice of the factorization point Q_0^2 . In the case of taking $Q_0^2 = 20 \text{ GeV}^2$ the NNLO perturbative QCD contributions are less important, than in the case $Q_0^2 = 5 \text{ GeV}^2$, previously considered in Ref.[11]. Indeed, for different Q^2 -cuts they are changing slightly the NLO values of $\Lambda_{\overline{MS}}^{(4)}$, provided twist-4 corrections are switched off.
- As was mentioned previously, this effect might be related to the peculiar behaviour of the NNLO perturbative expression for the $n = 2$ moment of the xF_3 SF (see Eq.(29)) and, therefore, to the theoretical uncertainty of the NNLO behaviour of the xF_3 SF at small x . We have checked this conclusion by comparing the results of the NLO and NNLO $Q_0^2 = 5 \text{ GeV}^2$ -fits of the CCFR'97 data cut at $x > 0.04$. The result of these test-fits demonstrate the tendency, identical to the one revealed after moving the factorization scale to $Q_0^2 = 20 \text{ GeV}^2$, namely the minimization of the difference between the values of $\Lambda_{\overline{MS}}^{(4)}$, extracted at the NLO and NNLO.
- However, in the case when the IRR-model for the twist-4 corrections are included into the analysis, the effects of the NNLO corrections are still important and are decreasing both the value of $\Lambda_{\overline{MS}}^{(4)}$ and the IRR-model parameter A'_2 , making the first one almost identical

	γ - free			$\gamma = 0$ - fixed		
$Q^2 >$	$\Lambda_{\overline{MS}}^{(4)}$ (MeV)	A'_2 (HT)	χ^2 /points	$\Lambda_{\overline{MS}}^{(4)}$ (MeV)	A'_2 (HT) (GeV^2)	χ^2 /points
5 GeV^2	LO	-	113.1/86	241±35	-	121.7/86
		264±35	-	113.1/86	241±35	-
	NLO	-0.33±0.06	82.8/86	398±71	-0.31±0.08	121.7/86
		433±52	-	83.1/86	313±36	-
	NNLO	-0.12±0.06	81.8/86	341±36	-0.11±0.05	92.3/86
		369±45	-	77.0/86	314±35	-
	N ³ LO	-0.01±0.05	76.9/86	315±34	-0.02±0.05	86.3/86
		326±35	-	76.9/86	314±28	-
(n.e.)	-0.04±0.05	76.3/86	315±27	-0.04±0.05	85.7/86	
	333±27	-	77.9/86	328±37	-	85.1/86
N ³ LO	-0.04±0.05	77.2/86	335±37	-0.05±0.05	84.2/86	
340±37	-	77.2/86	335±37	-0.05±0.05	84.2/86	
10 GeV^2	LO	-	77.3/63	283±39	-	78.1/63
		287±42	-0.52±0.12	57.8/63	515±75	-0.50±0.12
	NLO	-	63.9/63	344±44	-	64.8/63
		529±77	-0.24±0.10	58.3/63	427±55	-0.23±0.10
	NNLO	-	57.4/63	337±40	-	58.7/63
		349±40	-0.06±0.09	56.9/63	352±42	-0.03±0.09
	N ³ LO	-	57.3/63	347±41	-	58.0/63
		354±45	-0.09±0.09	56.2/63	373±48	-0.09±0.09
(n.e.)	-	56.8/63	345±30	-	57.3/63	
	373±48	-0.07±0.09	56.2/63	363±46	-0.07±0.09	56.6/63
N ³ LO	-0.07±0.09	56.2/63	363±46	-0.07±0.09	56.6/63	
362±46	-	56.2/63	363±46	-0.07±0.09	56.6/63	
15 GeV^2	LO	-	58.5/50	320±47	-	58.5/50
		319±48	-0.56±0.18	49.9/50	525±45	-0.56±0.20
	NLO	-	52.3/50	366±46	-	52.3/50
		530±89	-0.25±0.17	50.3/50	438±69	-0.24±0.17
	NNLO	-	50.4/50	341±44	-	50.8/50
		365±46	-0.03±0.15	50.3/50	347±55	-0.03±0.15
	N ³ LO	-	50.3/50	348±45	-	50.4/50
		440±71	-0.04±0.14	50.2/50	357±56	-0.04±0.15
(n.e.)	-	50.2/50	343±41	-	50.3/50	
	343±44	-0.02±0.15	50.2/50	347±54	-0.02±0.15	50.2/50
N ³ LO	-0.02±0.15	50.2/50	347±54	-0.02±0.15	50.2/50	
347±58	-	50.2/50	347±54	-0.02±0.15	50.2/50	

Table 4. The results of the extractions of the parameter $\Lambda_{\overline{MS}}^{(4)}$ and the IRR coefficient A'_2 , (in GeV^2) defined in Eq.(23), from LO, NLO, NNLO and N³LO non-expanded (n.e.) and expanded Padé fits of CCFR'97 data. In the fits $Q_0^2=20 GeV^2$

to the NNLO value of $\Lambda_{\overline{MS}}^{(4)}$, obtained without twist-4 terms, and the latter one compatible with zero within statistical error bars. A similar feature was also observed in the case of the fits, made in Ref.[11] for the factorization point $Q_0^2 = 5 \text{ GeV}^2$. This property is confirming the foundation of Ref.[11] that the results of the NNLO fits are less sensitive to the parameter of the IRR-model of the twist-4 term. The similar conclusion was also recently made in Ref.[48] while comparing the experimental data for the DIS R-ratio with the available NNLO perturbative QCD results of Ref.[49], although the earlier analysis of the experimental data for this quantity with the different kind of HT model is still leaving room for the power suppressed behaviour [50, 51].

- The values of $\Lambda_{\overline{MS}}^{(4)}$, which are coming from the fits taking into account the [0/2] Padé estimates (both in the expanded and non-expanded variants) turn out to be almost insensitive to the choice of the Q^2 -cut of the data, the value of γ and thus incorporation of the $(1 + \gamma x)$ -factor in the parton distribution model. The latter fact, in its turn, can indicate that the change of the model $x F_3(x, Q_0^2) = A(Q_0^2) x^{b(Q_0^2)} (1 - x)^{c(Q_0^2)} (1 + \gamma(Q_0^2)) x$ to $x F_3(x, Q_0^2) = A(Q_0^2) x^{b(Q_0^2)} (1 - x)^{c(Q_0^2)} (1 + \gamma(Q_0^2) x + \epsilon(Q_0^2) \sqrt{x})$, used in the MRST and GRV fits, might affect the obtained results only slightly;
- The large errors in the definite results for $\Lambda_{\overline{MS}}^{(4)}$, presented in Table 4, are reflecting the correlations of these uncertainties with the errors of the IRR-model parameter A'_2 ;
- The property $\chi_{LO}^2 > \chi_{NLO}^2 > \chi_{NNLO}^2 \sim \chi_{N^3LO}^2$ is reflecting the importance of taking into account the effects of higher order perturbative QCD corrections in the process of the fits of the concrete experimental data;
- For all Q^2 -cuts the expanded N³LO results for $\Lambda_{\overline{MS}}^{(4)}$ are almost identical to the ones obtained using the expansion of the Padé approximants in Taylor series. Moreover, the χ^2 -criterion do not discriminate between these two variants of the Padé motivated fits (see especially the results, obtained for the cuts $Q^2 > 10 \text{ GeV}^2$ and $Q^2 > 15 \text{ GeV}^2$). In our future studies we will consider the results of applications of the expanded Padé approximants.

The results of the NNLO Jacobi polynomials expansions fits are compared to the available CCFR'97 data in Fig.1. Drawing the theoretical curves we used Eq.(24) with zero twist-4 contributions. The value of the QCD scale parameter, which governs the theoretical behaviour of the moments of $x F_3$ SF, turned out to be $\Lambda_{\overline{MS}}^{(4)} = 326 \pm 35 \text{ MeV}$ (the χ^2 of the corresponding fits is 77.0/86). The values of the corresponding parameters of the $x F_3$ SF model at $Q_0^2 = 20 \text{ GeV}^2$ are : $A = 4.70 \pm 0.34$, $b = 0.65 \pm 0.03$, $c = 3.88 \pm 0.08$, $\gamma = 0.80 \pm 0.28$. One can see, that the NNLO results of the fits without twist-4 corrections are in good agreement with the CCFR'97 experimental data for the $x F_3$ SF.

In order to determine now the values of $\alpha_s(M_Z)$, we transformed $\Lambda_{\overline{MS}}^{(4)}$ through the threshold of the production of the fifth flavour, M_5 , using the LO, NLO, NNLO and N³LO variants of the rigorous \overline{MS} -scheme matching conditions, derived in Ref.[29] following the lines of Ref.[23]. The related values of $\Lambda_{\overline{MS}}^{(5)}$ can be obtained with the help of the following equation:

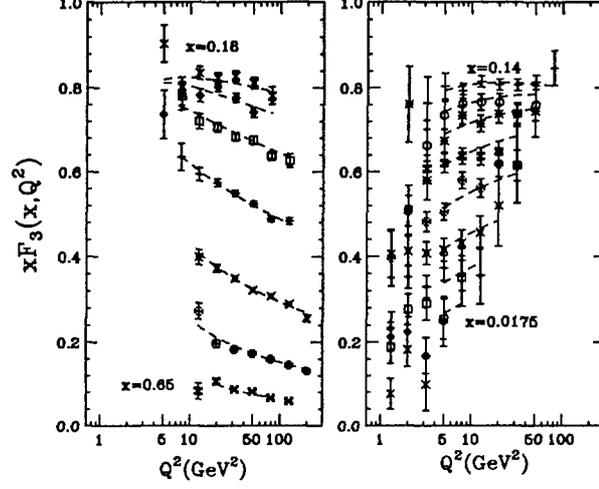


Fig.1 The comparison of the CCFR'97 data with the results of our NNLO Jacobi polynomial fits.

$$\beta_0^{f+1} \ln \frac{\Lambda_{\overline{MS}}^{(f+1)2}}{\Lambda_{\overline{MS}}^{(f)2}} = (\beta_0^{f+1} - \beta_0^f) L_h + \delta_{NLO} + \delta_{NNLO} + \delta_{N^3LO} \quad (30)$$

$$\delta_{NLO} = \left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} - \frac{\beta_1^f}{\beta_0^f} \right) \ln L_h - \frac{\beta_1^{f+1}}{\beta_0^{f+1}} \ln \frac{\beta_0^{f+1}}{\beta_0^f} \quad (31)$$

$$\delta_{NNLO} = \frac{1}{\beta_0^f L_h} \left[\frac{\beta_1^f}{\beta_0^f} \left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} - \frac{\beta_1^f}{\beta_0^f} \right) \ln L_h + \left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} \right)^2 - \left(\frac{\beta_1^f}{\beta_0^f} \right)^2 - \frac{\beta_2^{f+1}}{\beta_0^{f+1}} + \frac{\beta_2^f}{\beta_0^f} - C_2 \right] \quad (32)$$

$$\delta_{N^3LO} = \frac{1}{(\beta_0^f L_h)^2} \left[-\frac{1}{2} \left(\frac{\beta_1^f}{\beta_0^f} \right)^2 \left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} - \frac{\beta_1^f}{\beta_0^f} \right) \ln^2 L_h + \frac{\beta_1^f}{\beta_0^f} \left[-\frac{\beta_1^{f+1}}{\beta_0^{f+1}} \left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} - \frac{\beta_1^f}{\beta_0^f} \right) + \frac{\beta_2^{f+1}}{\beta_0^{f+1}} - \frac{\beta_2^f}{\beta_0^f} + C_2 \right] \ln L_h + \frac{1}{2} \left(-\left(\frac{\beta_1^{f+1}}{\beta_0^{f+1}} \right)^3 - \left(\frac{\beta_1^f}{\beta_0^f} \right)^3 - \frac{\beta_3^{f+1}}{\beta_0^{f+1}} + \frac{\beta_3^f}{\beta_0^f} \right) + \frac{\beta_1^{f+1}}{\beta_0^{f+1}} \left(\left(\frac{\beta_1^f}{\beta_0^f} \right)^2 + \frac{\beta_2^{f+1}}{\beta_0^{f+1}} - \frac{\beta_2^f}{\beta_0^f} + C_2 \right) - C_3 \right] \quad (33)$$

where $C_2 = -7/24$ was calculated in Ref.[27] (see also Erratum to Ref.[23]) and the analytic expression for C_3 , namely $C_3 = -(80507/27648)\zeta(3) - (2/3)\zeta(2)((1/3)\ln 2 + 1) - 58933/124416 + (f/9)[\zeta(2) + 2479/3456]$ was recently found in Ref.[29]. Here β_i^f (β_i^{f+1}) are the coefficients of the β -function with f ($f+1$) numbers of active flavours, $L_h = \ln(M_{f+1}^2/\Lambda_{\overline{MS}}^{(f)2})$ and M_{f+1} is the threshold of the production of the quark of the $(f+1)$ flavour. In our analysis we will take

$f = 4$ and $m_b \approx 4.8 \text{ GeV}$ and will vary the threshold of the production of the fifth flavour from $M_5^2 = m_b^2$ to $M_5^2 = (6m_b)^2$ in accordance with the proposal of the work of Ref.[26]. The difference between different prescriptions of fixing of matching point will be included into the estimate of the theoretical uncertainties of the final results for $\alpha_s(M_Z)$.

In the case of the non-zero values of the twist-4 function $h(x) \neq 0$, the results of the fits are presented in Table 5 in the next Section.

It should be stressed that we are considering the outcomes of our N³LO approximate fits as the theoretical uncertainties of the NNLO results in the same manner like the results of the NNLO analysis will be considered as the measure of theoretical uncertainties of the NLO results. In particular, we will introduce the characteristic deviations $\Delta^{NNLO} = |(\Lambda_{\overline{MS}}^{(4)})^{N^3LO} - (\Lambda_{\overline{MS}}^{(4)})^{NNLO}|$, $\Delta^{NLO} = |(\Lambda_{\overline{MS}}^{(4)})^{NNLO} - (\Lambda_{\overline{MS}}^{(4)})^{NLO}|$.

In the case when the twist-4 terms are included into the fits the difference $\Delta^{NNLO} = |(\Lambda_{\overline{MS}}^{(4)})^{N^3LO} - (\Lambda_{\overline{MS}}^{(4)})^{NNLO}|$ is smaller than the NLO correction term $\Delta^{NLO} = |(\Lambda_{\overline{MS}}^{(4)})^{NNLO} - (\Lambda_{\overline{MS}}^{(4)})^{NLO}|$. The similar tendency $\Delta^{NNLO} < \Delta^{NLO}$ is taking place in the case of the fits without twist-4 corrections. These observed properties demonstrate the reduction of the theoretical errors due to cutting the analyzed perturbation series at the different orders.

It is known that the inclusion of the higher-order perturbative QCD corrections in the procedures of the comparison with the experimental data is decreasing the scale-scheme theoretical errors of the results for $\Lambda_{\overline{MS}}^{(4)}$ and thus $\alpha_s(M_Z)$ (see e.g. Refs.[52, 18, 34]). Among the ways of probing the scale-scheme uncertainties are the scheme-invariant methods, namely the principle of minimal sensitivity, the effective charges approach (which is known to be identical to the scheme-invariant perturbation theory) and the BLM approach (for a review of these methods see e.g. Ref.[53]). The scheme-invariant methods were already used to estimate the effects of the unknown higher order corrections in SFs (see Ref.[51], where a strong decrease of the value of the QCD scale parameter was found in the process of the NLO scheme-invariant fit of the experimental data for the NS part of the F_2 SF). It was also used to try to estimate the unknown at present N³LO corrections to the definite physical quantities [36], and DIS sum rules among others. Note that the predictions of Ref.[36] turned out to be in agreement with the results of applications of the Padé resummation technique (see Ref.[33]). Therefore, we can conclude that the application of the methods of the Padé approximants should lead to the reduction of the scale-scheme dependence uncertainties of the values of $\alpha_s(M_Z)$ in the analysis of the CCFR data.

In order to consider the applicability of the Padé resummation technique for fixing scale-scheme dependence ambiguities, we performed the scheme-invariant fits following the ideas of Ref.[54]. We found that at the NNLO the application of the effective charges approach gave a rather high value of χ^2 ($\chi^2 \sim 111/86$). This, in a turn, can be related to the appearance of the *large* and *positive* values of the NNLO terms $\beta_2(n)_{eff}$ of the effective-charges β -functions, which are the important ingredients of the scheme-invariant approach of Ref.[54]. Similar problems have also been observed in the case of the scheme-invariant applications to the study of the NNLO perturbative QCD predictions to other renormalization-group invariant quantities (see Refs.[55, 41, 56] for discussions). In this work we will avoid the detailed investigation of this paradox. At the current level of our understanding we think that the described peculiar features of the effective-charges approach gives the support to the application of [0/2] Padé resummation technique for fixing scale-scheme dependence ambiguities of the results of the NNLO analysis of the CCFR'97 experimental data.

We are presenting now the values of $\alpha_s(M_Z)$, extracted from the fits of the CCFR'97 experimental data for the xF_3 SF, obtained with twist-4 contribution, modeled through the IRR model of Ref.[19]:

$$\begin{aligned} \text{NLO HT of Ref. [19]} \alpha_s(M_Z) &= 0.120 \pm 0.003(\text{stat}) \\ &\pm 0.005(\text{syst}) \pm 0.004(\text{theory}) \end{aligned} \quad (34)$$

$$\begin{aligned} \text{NNLO HT of Ref. [19]} \alpha_s(M_Z) &= 0.118 \pm 0.002(\text{stat}) \\ &\pm 0.005(\text{syst}) \pm 0.003(\text{theory}) . \end{aligned} \quad (35)$$

Anticipating the considerations of Sec.3(b) we also present the results of NLO and NNLO extractions of $\alpha_s(M_Z)$ with twist-4 contribution, modeled by the additional free parameters of the fit:

$$\begin{aligned} \text{NLO HT free } \alpha_s(M_Z) &= 0.123_{-0.010}^{+0.008}(\text{stat}) \\ &\pm 0.005(\text{syst}) \pm 0.004(\text{theory}) \end{aligned} \quad (36)$$

$$\begin{aligned} \text{NNLO HT free } \alpha_s(M_Z) &= 0.121_{-0.009}^{+0.007}(\text{stat}) \\ &\pm 0.005(\text{syst}) \pm 0.003(\text{theory}) . \end{aligned} \quad (37)$$

The systematic uncertainties are taken from the CCFR experimental analysis, presented in the first work of Ref.[2], and the theoretical uncertainties in the results of Eqs.(34),(36) [Eqs.(35),(37)] are estimated by the differences between the central values of the outcomes of the NNLO and NLO [N³LO and NNLO] fits, presented in Tables 4,5, plus the arbitrariness in the choice of the factorization scale and in the application of the \overline{MS} -scheme matching condition (which following the considerations of Ref.[26] was estimated as $\Delta\alpha_s(M_Z) = \pm 0.002$). In the process of fixing the theoretical errors with the consideration of the N³LO corrections we take into account the differences between the applications of the expanded and non-expanded Padé approximants.

It can be seen that due to the large overall number of the fitted parameters the results of Eqs.(36),(37) for $\alpha_s(M_Z)$ are receiving large statistical uncertainties. As can be seen from the results of Eq.(34),(35) for the QCD coupling constant, it is possible to decrease their values by fixing the concrete form of the twist-4 parameter $h(x)$. However, if one is interested in the extraction of the form of the twist-4 parameter $h(x)$, one should take for granted these intrinsic theoretical uncertainties of the value of $\alpha_s(M_Z)$.

3 (b). The analysis of the experimental data: the extraction of the shape of the twist-4 terms.

Apart from the perturbative QCD contributions, the expressions for DIS structure functions should contain the power-suppressed high-twist terms, which reflect the possible non-perturbative QCD effects. The studies of these terms have a rather long history. At the beginning of these studies it was realized that the twist-4 contributions to structure functions should have the pole-like behavior $\sim 1/((1-x)Q^2)$ [57, 58]. This behavior was used in the phenomenological investigations of the earlier less precise DIS νN data [59, 60, 61], which together with other different procedures of analyzing neutrino DIS data [62, 63] was considered as the source of the information about scaling violation parameters. The development of the renormalon technique (Refs.[21, 19, 20] and Ref.[22] for the detailed review) pushed ahead the more detailed phenomenological analysis of the possibility of detecting higher-twist components in the most precise DIS data available at present, obtained by BCDMS, SLAC, CCFR and other collaborations. It turned out that despite the qualitative status of the renormalon approach, the satisfactory description of the results of the QCD NLO F_2 SF analysis [64] in terms of the IRR technique was achieved [19, 21]. The next step was to clarify the status of the predictions of

Ref.[19] for the form and sign of the twist-4 contributions to xF_3 SF. The study of this problem was done in Ref.[11] (see also Ref.[10]). In this section we are discussing the results of a more refined analysis of the behavior of the twist-4 contributions to xF_3 SF at the LO, NLO, NNLO and beyond.

In Table 4 we study the dependence of the extracted value of the parameter A'_2 from the different orders of perturbative QCD predictions, Q^2 -cuts of the CCFR experimental data and the coefficient γ of parton distributions model for xF_3 , fixing the factorization scale $Q_0^2 = 20 \text{ GeV}^2$. Note, that the parameter A'_2 was introduced in the IRR model of Eq.(28), taken from Ref.[19], and fixed there as $A'_2 \approx -0.2 \text{ GeV}^2$, which is necessary for the description of the fitted twist-4 results of Ref.[64] for the F_2 SF within the IRR language. We found that the value of this parameter, extracted at the LO and NLO, is negative, differs from zero for about one standard deviation and qualitatively agrees with the IRR-motivated guess of Ref.[19]. Moreover, the results of our LO and NLO fits are also in agreement with the value of the parameter $h = -0.38 \pm 0.06 \text{ GeV}^2$ of the different model of the twist-4 contribution to xF_3 , namely $xF_3(x, Q^2)h/((1-x)Q^2)$, extracted previously in Ref.[61] from the old νN DIS data.

It is interesting to notice that the results of Table 4 reveal that for larger Q^2 -cuts 10–15 GeV^2 the values of A'_2 in the LO and NLO fits are less sensitive to the included number of the experimental points than in the case of the low Q^2 cut (5 GeV^2). This feature can be related to the logarithmic increase of the QCD coupling constant A_s at lower Q^2 . However, since we are interested in the extraction of the power-suppressed twist-4 contribution, we shall concentrate on the discussion of the more informative, from our point of view, fits with low Q^2 -cut 5 GeV^2 , which contain more experimental points and thus are more statistically motivated.

We are now turning to the pure phenomenological extraction of the twist-4 contribution $h(x)$ to xF_3 (see Eq.(24)), which is motivated by the work of Ref.[64] for the F_2 SF. In the framework of this approach the x -shape of $h(x)$ is parametrized by the additional parameters $h_i = h(x_i)$, where x_i are the points of the experimental data binning. The results of the multiloop extractions of these parameters are presented in Table 5 and are illustrated by the curves of Fig.2.

	LO	NLO	NNLO	N ³ LO (Pade)
$\chi_{d.f.}^2$	66.3/86	65.7/86	65.0/86	64.8/86
A	5.33 ± 1.33	4.71 ± 1.14	4.79 ± 0.75	5.14 ± 0.73
b	0.69 ± 0.08	0.66 ± 0.08	0.66 ± 0.05	0.68 ± 0.05
c	4.21 ± 0.17	4.09 ± 0.14	3.95 ± 0.19	3.84 ± 0.23
γ	1.15 ± 0.94	1.34 ± 0.86	0.96 ± 0.57	0.57 ± 0.52
$\Lambda_{\overline{MS}}^{(4)} [MeV]$	331 ± 162	440 ± 183	372 ± 133	371 ± 127
x_i	$h(x_i) [GeV^2]$			
0.0125	0.209 ± 0.346	0.235 ± 0.325	0.263 ± 0.315	0.304 ± 0.313
0.0175	0.067 ± 0.281	0.114 ± 0.283	0.133 ± 0.263	0.170 ± 0.257
0.025	0.153 ± 0.215	0.242 ± 0.226	0.244 ± 0.206	0.268 ± 0.199
0.035	-0.013 ± 0.205	0.132 ± 0.236	0.112 ± 0.211	0.110 ± 0.195
0.050	0.038 ± 0.159	0.256 ± 0.240	0.214 ± 0.200	0.171 ± 0.168
0.070	-0.141 ± 0.139	0.144 ± 0.258	0.106 ± 0.202	0.017 ± 0.151
0.090	-0.177 ± 0.127	0.144 ± 0.254	0.142 ± 0.202	0.026 ± 0.142
0.110	-0.343 ± 0.127	-0.009 ± 0.237	0.045 ± 0.205	-0.080 ± 0.146
0.140	-0.408 ± 0.116	-0.085 ± 0.174	0.060 ± 0.187	-0.049 ± 0.140
0.180	-0.351 ± 0.173	-0.072 ± 0.128	0.154 ± 0.161	0.093 ± 0.145
0.225	-0.547 ± 0.244	-0.351 ± 0.180	-0.098 ± 0.128	-0.103 ± 0.127
0.275	-0.548 ± 0.334	-0.472 ± 0.321	-0.228 ± 0.185	-0.193 ± 0.169
0.350	-0.295 ± 0.414	-0.390 ± 0.470	-0.154 ± 0.264	-0.104 ± 0.234
0.450	-0.098 ± 0.410	-0.307 ± 0.504	-0.146 ± 0.330	-0.125 ± 0.303
0.550	0.095 ± 0.324	-0.134 ± 0.415	-0.121 ± 0.323	-0.138 ± 0.317
0.650	0.380 ± 0.211	0.215 ± 0.262	0.140 ± 0.245	0.111 ± 0.251

Table 5. The results of the extractions of the HT contribution $h(x)$ to xF_3 and the parameters A, b, c, γ with the corresponding statistical errors. The QCD fits of the CCFR'97 data were performed taking into account TMC at the LO, NLO ($N_{max} = 10$), NNLO and N³LO ($N_{max} = 6$). In the latter case the expanded [0/2] Padé approximants were used. The fits are done for $Q_0^2 = 20 GeV^2$.

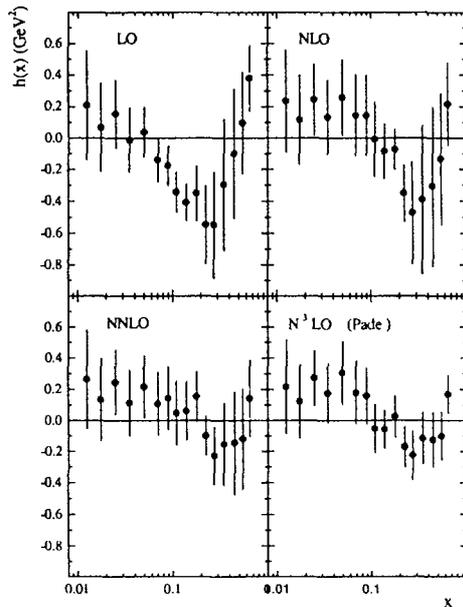


Fig.2. The x -shape of $h(x)$ extracted from the fits of the CCFR'97 data in the case of fixing the factorization point at $Q_0^2 = 20 \text{ GeV}^2$

Looking carefully at Table 5 and Fig.2 we observe the following features:

1. The x -shape of the twist-4 parameter is not inconsistent with the expected rise of $h(x)$ for $x \rightarrow 1$ [57, 58] in all orders of perturbation theory;
2. the values of the parameters $h(x_i)$ at the upper and lower points of kinematic region ($x_{16}=0.650$ and $x_1=0.0125$) are stable to the inclusion of the higher order perturbative QCD corrections and application of the Padé resummation technique. At large values of x this feature is in agreement with the previous statement;
3. the function $h(x)$ seems to cross zero twice: at small x of order 0.03 and larger x about 0.4. It should be noted that the sign-alternating behavior of the twist-4 contributions to DIS structure functions was qualitatively predicted in Ref.[60];
4. In the LO and NLO our results are in qualitative agreement with the IRR prediction of Ref.[19] (for discussions see Ref.[22]);
5. In the NNLO this agreement is not so obvious, though a certain tendency of the manifestation of the remaining structure of the twist-4 term is surviving even at the NNLO;
6. however, at the NNLO we observe the minimization of the amplitude of the $h(x)$ -variation. Thus we conclude that the inclusion of the NNLO corrections into the game might "shadow" the effects of the power suppressed terms at the NNLO. This property was previously observed at the LO as a result of the analysis of the less precise DIS neutrino data in Ref.[59]. In the modern experimental situation, namely in the process of the analysis of the more precise DIS neutrino data of the CCFR collaboration, we are observing this feature at the NNLO;

7. we checked the reliability of the foundation of the minimization of the amplitude of variation of $h(x)$ at the NNLO by going beyond this perturbative approximation using the method of Padé approximants. The result of this analysis reveals the relative stability of the NNLO results for $h(x)$;
8. the property of the minimization of the x -shape of $h(x)$ at the NNLO and N³LO is identical to the effect of decreasing of the IRR model parameter A_2' at the NNLO and N³LO (see Table 4);
9. these observed properties clarify why the results of the NNLO and N³LO fits for $\Lambda_{\overline{MS}}^{(4)}$, presented in Tables 4,5 practically do not depend from the inclusion of the twist-4 contribution through the IRR model. Indeed, at this level the twist-4 terms are manifesting themselves less obviously.

In our point of view, the foundations (8)-(9) reflect the selfconsistency of the results of our different fits with twist-4 terms included in different ways.

4. The quest of the inclusion of the effects of nuclear corrections.

The effects of nuclear corrections are the remaining important source of the uncertainties of the analysis of the DIS data. This is especially important for the experiments on heavy targets and in the case of CCFR data—on iron ⁵⁶Fe.

The attempts to study these effects were done in Ref.[65] in the framework of Deuteron-motivated model. The satisfactory QCD description of the CCFR data for xF_3 was achieved due to the reason that in this case the nuclear effects do not exceed 5 % effect. However, the more realistic description of nuclear effect for the xF_3 SF in the case of ⁵⁶Fe-target [66] revealed the appearance of new $1/Q^2$ and $1/M$ corrections for the NS moments (where M is the mass of the nucleon), which have the following form

$$\begin{aligned}
M_n^A(Q^2)/A &= \left(1 + \frac{\epsilon}{M}(n-1) + \frac{\langle \mathbf{p}^2 \rangle}{6M^2}n(n-1) + O\left(\frac{1}{M^3}\right)\right) M_n^{NS}(Q^2) \\
&+ \langle \Delta p^2 \rangle \partial_{p^2} M_n^{NS}(Q^2) \\
&+ \frac{2 \langle \mathbf{p}^2 \rangle}{3Q^2} n(n+1) M_{n+2}^{NS}(Q^2)
\end{aligned} \tag{38}$$

where for ⁵⁶Fe the parameters of the nuclear model, adopted in Ref.[66] are $\langle \epsilon \rangle \approx -56 \text{ MeV}$, $\langle \mathbf{p}^2 \rangle / (2M) \approx 35 \text{ MeV}$, $\langle \Delta p^2 \rangle_{Fe} \approx -0.17 \text{ GeV}$ and the derivative $\partial_{p^2} M_n(Q^2)$ is taking into account that the target momentum p can be generally of-mass-shell. This effect is resulting in the following contribution [66]

$$\partial_{p^2} M_n(Q^2) = \partial_{p^2} M_n^{as} + \frac{n}{Q^2} \left(M_n^{NS} + M^2 \partial_{p^2} M_n^{as} \right) \tag{39}$$

which is independent from the nuclear content of the target. Note, that the numerical values of $\partial_{p^2} M_n^{as}$ were also presented in Ref.[66].

Note, that the effects of the nuclear corrections in DIS were also recently studied in Ref.[67] in the case of xF_3 SF and in Refs.[68],[69] in the case of F_2 SF (for the earlier related works see e.g. Ref.[70]). However, in our studies we will concentrate ourselves on the consideration of the results of Ref.[66].

We included the corrections of Eqs.(38)-(39) into our fits and observed the unacceptable increase of χ^2 value. We think that this can be related to the manifestation of the possible asymptotic character of the $1/M$ -expansion in Eq.(38), since the third term in the brackets of the r.h.s. of Eq.(38) becomes comparable with the first term (which is equal to unit) for the $n \sim 8$ used in our fits. Note that the moments with large n are important in the reconstruction

of the behavior of the xF_3 SF at $x \rightarrow 1$. This observed feature necessitates the derivation of the explicit expression for $M_n^A(Q^2)$, which is not expanded in powers of $1/M$ -terms. It should be added that the problem of the possible asymptotic nature of the power suppressed expansions was mentioned in the case of Ellis-Jaffe and Bjorken DIS sum rules in Ref.[71].

Another possibility to explain the non-convergence of our fits with the nuclear corrections of Eq.(38) taken into account might be related to the fact that the parton distribution model for the nuclear SF xF_3^{56Fe} can be different from the canonical model, used by us[72]. In any case, we think that the study of the problem of the possible influence of the heavy nuclear effects on the results of fits of xF_3 data is still on the agenda.

Conclusion

In this work we presented the results of the extractions of $\alpha_s(M_Z)$ and twist-4 terms from the QCD analysis of the CCFR data taking into account definite QCD corrections at the NNLO and beyond. Within experimental and theoretical errors our results for $\alpha_s(M_Z)$ are in agreement with other extractions of this fundamental parameter, including its world average value $\alpha_s(M_Z) = 0.118 \pm 0.005$.

Our estimate of the NNLO theoretical uncertainties is based on application of the [0/2] Padé approach at the N^3 LO level. The uncertainties of our NNLO analysis can be decreased after explicit NNLO calculations of the NS Altarelli-Parisi kernel. It should be added, however, that the obtained by us NLO results both for the x -shape of the twist-4 corrections and for the $\alpha_s(M_Z)$ value are in good agreement with the results of the NLO DGLAP analysis of the CCFR'97 xF_3 and F_2 SFs data [73], which gives $\alpha_s(M_Z) = 0.1222 \pm 0.0048$ (*exp*) ± 0.0040 (*theor*)

As to the twist-4 term, we found that despite the qualitative agreement of our NLO results with the IRR model prediction, at the NNLO level its x -shape has the tendency to decrease and is stable to the application of the [0/2] Padé motivated N^3 LO analysis.

This feature can be related to the fact that the analysis of the CCFR data cannot distinguish the twist-4 $1/Q^2$ terms from the NNLO perturbative QCD approximations of the Mellin moments. This possible explanation is similar to the conclusions of the LO analysis of the old less precise neutrino DIS data, made by the authors of Ref.[59]. It is worth to remind that they were unable to distinguish between LO logarithmic and $1/Q^2$ -behavior of the QCD contributions to Mellin moments of xF_3 . The experimental precision achieved in our days might move this effect to the NNLO. Another possibility is that the inclusion of the NNLO perturbative QCD contributions are making the extraction of the $1/Q^2$ -corrections both within IRR model approach and by the model-independent way more problematic (for a discussions of the perturbatively based alternative of the IRR language within quantum mechanics model see Ref.[74]).

Another related explanation is that the NNLO effect observed by us is manifesting itself in view of the fact that the twist-4 terms detected by us might come from the partial summation of the definite terms of the asymptotic perturbative QCD series and thus the increase of the order of perturbative QCD analysis effectively suppresses the remaining sum of the perturbative QCD contribution. One can hope that a future experiments of NuTeV collaboration will allow one to get the new experimental data at the precision level, necessary for extracting more detailed information about the higher twist contributions.

Note added

After the technical part of this work was done we learned about the work of Ref.[75] where the NNLO analysis of the F_2 SLAC, HERA and BCDMS data was performed both in the singlet and nonsinglet cases with the help of the method of Bernstein polynomials [76]. The main result of this work is the NNLO value $\alpha_s(M_Z) = 0.1163 \pm 0.0023$, which is in agreement with our findings. In another recent work the first steps towards the inclusion of the NNLO corrections to the NS part of F_2 SF and modeling the NNLO corrections to the kernel in the x -space were made [77]. We hope that our possible future studies will allow to generalize the Jacobi polynomial NNLO analysis presented in this work to the case of F_2 SF also.

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