

The APFEL DIS Module

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Abstract

In this document I will describe the old and the new DIS module embedded in APFEL.

Contents

1	Computing DIS Structure Functions on a Grid: the New DIS Module	2
1.1	Zero Mass Structure Functions	2
1.1.1	Coefficient Functions Treatment	3
1.2	Massive Structure Functions	4
1.2.1	Neutral Current Coefficient Functions	5
1.2.2	Charged Current Coefficient Functions	6
2	Target Mass Corrections	11
3	Renormalization and Factorization Scale Variation	13
4	Implementation of the Semi-Inclusive e^+e^- Annihilation	22
5	Polarized DIS cross section and structure functions	23
6	The χ Prescription in FONLL	24

1 Computing DIS Structure Functions on a Grid: the New DIS Module

In order to speed up and optimize the computation of the DIS structure functions in APFEL we decided to use the same technology used for the PDF evolution. In fact, up to version 2.0.0, the computation of such observables in APFEL was performed by directly convoluting PDFs with the coefficient functions by mean of a numerical integration.

Now the aim is that of precomputing on a grid the convolution of the coefficient functions with a set of interpolating polynomials. This way, the time consuming task of precomputing the coefficient functions of the grid needs to be done only once and the numerical convolution with any PDF set is instead very fast. In addition, as we will see below, this approach provides a very natural framework to combine precomputed coefficient functions and evolution operators, so that any prediction of structure functions at any scale Q can be obtained very quickly by convolution with PDFs at some initial scale Q_0 . Ultimately, this is particularly suitable for PDF fits.

1.1 Zero Mass Structure Functions

A structure function in the Zero-Mass (ZM) scheme is given by the following convolution:

$$F(x, Q) = \sum_{i=g,q} x \int_x^1 \frac{dy}{y} C_i \left(\frac{x}{y}, \alpha_s(Q) \right) q_i(y, Q), \quad (1.1)$$

Now, defining $t = \ln(Q^2)$, $\tilde{C}_i^{(n)}(y, t) = y C_i^{(n)}(y, \alpha_s(Q))$ and $\tilde{q}_i(y, t) = y q_i(y, Q)$, the integral above can be written as:

$$F(x, t) = \sum_{i=g,q} \int_x^1 \frac{dy}{y} \tilde{C}_i \left(\frac{x}{y}, t \right) \tilde{q}_i(y, t). \quad (1.2)$$

But, using a suitable interpolation basis, we can write:

$$\tilde{q}_i(y, t) = \sum_{\alpha=0}^{N_x} w_{\alpha}^{(k)}(y) \tilde{q}_i(x_{\alpha}, t), \quad (1.3)$$

so that eq. (1.2) becomes:

$$F(x, t) = \sum_{i=g,q} \sum_{\alpha=0}^{N_x} \left[\int_x^1 \frac{dy}{y} \tilde{C}_i \left(\frac{x}{y}, t \right) w_{\alpha}^{(k)}(y) \right] \tilde{q}_i(x_{\alpha}, t). \quad (1.4)$$

Now let's assume that x is on the grid, so that $x = x_{\beta}$. This way we have:

$$F(x_{\beta}, t) = \sum_{i=g,q} \sum_{\alpha=0}^{N_x} \underbrace{\left[\int_{x_{\beta}}^1 \frac{dy}{y} \tilde{C}_i \left(\frac{x_{\beta}}{y}, t \right) w_{\alpha}^{(k)}(y) \right]}_{\Gamma_{i,\beta\alpha}(t)} \tilde{q}_i(x_{\alpha}, t). \quad (1.5)$$

Using the same arguments presented in the evolution code notes, we have that:

$$\Gamma_{i,\beta\alpha}(t) \neq 0 \quad \text{for} \quad \beta \leq \alpha, \quad (1.6)$$

and:

$$\Gamma_{i,\beta\alpha}(t) = \int_c^d \frac{dy}{y} \tilde{C}_i(y, t) w_{\alpha}^{(k)} \left(\frac{x_{\beta}}{y} \right) \quad (1.7)$$

with:

$$c = \max(x_{\beta}, x_{\beta}/x_{\alpha+1}) \quad \text{and} \quad d = \min(1, x_{\beta}/x_{\alpha-k}). \quad (1.8)$$

The same symmetries holding for the splitting function case hold also here.

1.1.1 Coefficient Functions Treatment

The structure of the DIS coefficient functions is very similar to that of splitting functions with only one small complication, that is the presence of a more divergent singular term. In practice the structure of the DIS coefficient functions is the following:

$$\tilde{C}_i(x, t) = xC_i^R(x, t) + xC_i^{S1}(t) \left[\frac{1}{1-x} \right]_+ + xC_i^{S2}(t) \left[\frac{\ln(1-x)}{1-x} \right]_+ + xC_i^L(t)\delta(1-x). \quad (1.9)$$

The term proportional to C_i^{S2} can be treated, considering that:

$$\begin{aligned} \int_c^d dy \left[\frac{\ln(1-y)}{1-y} \right]_+ f(y) &= \int_c^d dy \frac{\ln(1-y)}{1-y} [f(y) - f(1)\theta(d-1)] \\ &+ \frac{1}{2} f(1) \ln^2(1-c)\theta(d-1) \end{aligned} \quad (1.10)$$

On the same line of splitting functions, we know that the coefficient functions ha the following perturbative expansion:

$$C_i^J(x, t) = \sum_{n=0}^N a_s^n(t) C_i^{J,(n)}(x) \quad \text{with} \quad J = R, S1, S2, L \quad (1.11)$$

Therefore one has that:

$$\begin{aligned} \Gamma_{j,\beta\alpha}(t) &= \sum_{n=0}^N a_s^n(t) \left\{ \int_c^d dy \left[C_i^{R,(n)}(y) w_\alpha \left(\frac{x_\beta}{y} \right) + \frac{C_i^{S1,(n)} + C_i^{S2,(n)} \ln(1-y)}{1-y} \left(w_\alpha \left(\frac{x_\beta}{y} \right) - \delta_{\beta\alpha} \theta(d-1) \right) \right] \right. \\ &\quad \left. + \left[C_i^{S1,(n)} \ln(1-c)\theta(d-1) + \frac{1}{2} C_i^{S2,(n)} \ln^2(1-c)\theta(d-1) + C_i^{L,(n)} \right] \delta_{\beta\alpha} \right\}. \end{aligned} \quad (1.12)$$

Calling:

$$\begin{aligned} \Gamma_{i,\beta\alpha}^{(n)}(t) &= \int_c^d dy \left[C_i^{R,(n)}(y) w_\alpha \left(\frac{x_\beta}{y} \right) + \frac{C_i^{S1,(n)} + C_i^{S2,(n)} \ln(1-y)}{1-y} \left(w_\alpha \left(\frac{x_\beta}{y} \right) - \delta_{\beta\alpha} \theta(d-1) \right) \right] \\ &+ \left[C_i^{S1,(n)} \ln(1-c)\theta(d-1) + \frac{1}{2} C_i^{S2,(n)} \ln^2(1-c)\theta(d-1) + C_i^{L,(n)} \right] \delta_{\beta\alpha}, \end{aligned} \quad (1.13)$$

we have that:

$$\Gamma_{i,\beta\alpha}(t) = \sum_{n=0}^N a_s^n(t) \Gamma_{i,\beta\alpha}^{(n)}, \quad (1.14)$$

and the integrals $\Gamma_{i,\beta\alpha}^{(n)}$ do not depend on the energy therefore, once the grid (and the number of active flavours) has been fixed, they can be evaluate once and for all at the beginning and used for the convolution at any scale.

Now, assuming to have computed the evolution operator $M_{ij,\alpha\beta}(t, t_0)$ between the scales $t = \ln(Q^2)$ and $t_0 = \ln(Q_0^2)$ on the same grid where we have computed the operator $\Gamma_{i,\beta\alpha}(t)$, one can esily combine the two obtaining the prediction for the structure function F on the grid in terms of PDFs at the initial scale Q_0 just by performing the following convolution:

$$F(x_\alpha, t) = \Gamma_{i,\alpha\beta}(t) M_{ij,\beta\gamma}(t, t_0) \tilde{q}_j(x_\gamma, t_0) \quad (1.15)$$

where a sum of the repeated indeces is understood.

Before proceeding to treatment of the massive coefficient functions, we stress that in the massless scheme, for obviuos kinematical reasons, there is no need to distinguish between charged- and neutral-current coefficient functions. The difference between the two cases appears only at the level of structure functions where

the coefficient functions are convoluted with different combinations of PDFs and combined according to the structure of the couplings to quarks of the Z/γ^* vector bosons in the neutral-current case and the W^\pm in the charged-current case.

It is opportune at this point to mention that, when considering charged-current observables at NLO in the massive scheme, there is a further contribution to be added to eq. (1.9) that has the form:

$$C_i^{SL}(t) \frac{d}{dx} \delta(1-x). \quad (1.16)$$

Starting from the relation:

$$x \frac{d}{dx} \delta(x) = -\delta(x), \quad (1.17)$$

one can easily show that:

$$\frac{d}{dx} \delta(1-x) = \left[\frac{\delta(1-x)}{1-x} \right]_+. \quad (1.18)$$

To make sure that this identity is correct, we try to convolute both the r.h.s. and the l.h.s. of eq. (1.18) with the test function $f(x)$, such that $f(1) = 0$, to see what is the result and whether the results are equal. Using the l.h.s. we have:

$$\int_x^1 dy f(y) \frac{d}{dx} \delta(1-y) = \underbrace{f(y) \delta(1-y)}_{=0} \Big|_x^1 - \int_x^1 dy \frac{df(y)}{dy} \delta(1-y) = - \frac{df(y)}{dy} \Big|_{y=1}, \quad (1.19)$$

while using the r.h.s.⁽¹⁾:

$$\begin{aligned} \int_x^1 dy f(y) \left[\frac{\delta(1-y)}{1-y} \right]_+ &= \int_x^1 dy \frac{f(y) - f(1)}{1-y} \delta(1-y) = \lim_{\epsilon \rightarrow 0^+} \int_x^1 dy \frac{f(y) - f(1)}{1-y} \delta(1-\epsilon-y) = \\ &= - \lim_{\epsilon \rightarrow 0^+} \frac{f(1) - f(1-\epsilon)}{\epsilon} = - \frac{df(y)}{dy} \Big|_{y=1}. \end{aligned} \quad (1.20)$$

So the results are equal and the distributions in eq. (1.18) when convoluted with a test function extract its derivative in $y = 1$, up to a minus sign.

At the end of the day one has to include inside the curly brackets of eq. (1.12) the term:

$$- C_i^{SL,(n)} \frac{dw_\alpha^{(k)}(x_\beta)}{dx} \quad (1.21)$$

In addition, when using a Lagrange interpolation, one can show that the first derivative of the Lagrange polynomials have the form:

$$\frac{dw_\alpha^{(k)}(x_\rho)}{dx} = \begin{cases} \sum_{\substack{\sigma=0 \\ \sigma \neq \alpha}}^k \frac{1}{x_\alpha - x_\sigma} & \rho = \alpha \\ \frac{1}{x_\alpha - x_\rho} \prod_{\substack{\sigma=0 \\ \sigma \neq \alpha, \rho}}^k \frac{x_\rho - x_\sigma}{x_\alpha - x_\sigma} & \rho \neq \alpha \end{cases} \quad (1.22)$$

The relation in eq. (1.22) is proved in the “Lagrange_derivative.pdf” notes.

1.2 Massive Structure Functions

Now we can proceed considering the massive structure functions. When computing structure functions in the massive scheme, there is a further complication that complicates a fast precomputation of the coefficient functions on the x -space grid and it is the fact that the coefficients of the perturbative expansion of the massive

¹ Since the delta function selects the point $y = 1$ in the following integral, the “incomplete” integral of plus-prescribed function does not give rise to any residual logarithm of the form $\ln(1-x)$.

coefficient functions carry an intrinsic dependence on the scale of the process. This prevents a scale independent pre-tabulation of the coefficient functions on an x -space grid.

One possible way out is to pre-tabulate the coefficient functions, not only on an x -space grid, but also on a Q -space grid, where Q is the scale at which the structure functions are evaluated. Actually the most efficient way of precomputing the massive coefficient functions is on ξ -space grid, where ξ is defined as:

$$\xi = \frac{Q^2}{m_H^2}. \quad (1.23)$$

where m_H is the mass of the heavy quark under consideration. In fact, for dimensional reasons, massive coefficient functions depend on the scale Q through ξ . Neglecting for the moment the dependence on the renormalization and on the factorization scales, the massive coefficient functions allow for the following expansion:

$$C_i(x, Q, m_H) = \sum_n a_s^n(t) C_i^{(n)}(x, \xi). \quad (1.24)$$

Given this relation, the massive analogous of the eq. (1.14) is:

$$\Gamma_{i,\beta\alpha}(Q, m_H) = \sum_n a_s^n(t) \Gamma_{i,\beta\alpha}^{(n)}(\xi). \quad (1.25)$$

In order not to recompute the operator $\Gamma_{i,\beta\alpha}^{(n)}(\xi)$ any time that ξ changes, we can tabulate the on a grid in ξ , $\{\xi_1, \dots, \xi_\tau, \dots, \xi_{N_\xi}\}$, defining:

$$\Gamma_{i,\beta\alpha,\tau}^{(n)} = \Gamma_{i,\beta\alpha}^{(n)}(\xi_\tau), \quad (1.26)$$

and then interpolate to obtain the operator for a generic value of ξ . We have chosen to use a linear interpolation so that:

$$\Gamma_{i,\beta\alpha}^{(n)}(\xi) = c^{(0)}(\xi) \Gamma_{i,\beta\alpha,\tau}^{(n)} + c^{(1)}(\xi) \Gamma_{i,\beta\alpha,\tau+1}^{(n)}, \quad (1.27)$$

with:

$$c^{(0)}(\xi) = \frac{\ln \xi_{\tau+1} - \ln \xi}{\ln \xi_{\tau+1} - \ln \xi_\tau} \quad \text{and} \quad c^{(1)}(\xi) = \frac{\ln \xi - \ln \xi_\tau}{\ln \xi_{\tau+1} - \ln \xi_\tau}, \quad (1.28)$$

provided that $\xi_\tau \leq \xi < \xi_{\tau+1}$.

To conclude, once the operators $\Gamma_{i,\beta\alpha,\tau}^{(n)}$ have been precomputed, the operator for a generic value of ξ can be quickly computed by interpolation.

1.2.1 Neutral Current Coefficient Functions

As far as the neutral current coefficient functions are concerned, beyond $\text{LO}^{(2)}$, a close analytical form is not available and only a semi-analytical form [1] which is not suitable for a fast numerical implementation. The authors of Ref. [2] have used a simple parametrization to fit the exact coefficient functions. Such parametrization is actually meant to be used in Mellin space, however it can equally be used in x space providing a fast and accurate enough alternative to the original implementation. The parametrization of Ref. [2] has the form:

$$C(x, \xi) = \theta(\rho - x)(\rho - x)^{-\kappa} \sum_{k=0}^K a_k(\rho) x^k \quad \text{with} \quad \rho = \frac{\xi}{\xi + 4}, \quad (1.29)$$

and the authors provide the numerical values of κ , K and $a_k(\rho)$ for all the relevant coefficient functions at LO ($\mathcal{O}(\alpha_s)$) and NLO ($\mathcal{O}(\alpha_s^2)$) tabulated on a ξ -space grid for large enough range in ξ . Note the presence of the θ -function that has the scope of reducing the phase space available for the process due the production of two heavy quarks in the final state.

In APFEL we make use of the parametrization above only for the NLO coefficient functions as the exact form of the LO ones is available in Ref. [3] and compact enough for an efficient implementation. In addition, also for the pure singlet NLO coefficient functions (sometimes called gluon-radiation terms) we employ the analytical expressions given in Appendix A of Ref. [4].

We finally remark that massive coefficient functions for the neutral current structure functions are presently known only for F_2 and F_L . For the parity-violating structure function F_3 we thus use the massless coefficient functions.

² We remind that, in the neutral current case, the LO is order α_s .

As far as the massless limit of the massive (massive-zero) coefficient functions is concerned, exact expressions up to $\mathcal{O}(\alpha_s^2)$ have been evaluated in Ref. [4] and reported in Appendix D. Such expressions are implemented in APFEL

As in the massive case, massive-zero coefficient functions are known only for F_2 and F_L and again for the F_3 structure function we use the massless coefficient functions.

1.2.2 Charged Current Coefficient Functions

We can now consider the charged-current sector. In this case, massive coefficient functions are known only up to $\mathcal{O}(\alpha_s)$ (NLO), therefore a proper computation of charged-current structure functions the NNLO version of the FONLL scheme (called FONLL-C) is impossible. However, the best we can do when computing charged-current structure functions in the FONLL-C scheme is to set the NNLO contributions to zero in the massive sectors but keeping those in the massless sector, as well as using NNLO evolution for PDFs and α_s .

The charged-current massive structure functions, like the other structure functions, are given by the convolution of PDFs with coefficient functions. Considering the heavy-quark H structure functions in the approximation of diagonal CKM matrix, the definitions are:

$$F_1^H(x, Q, m_H) = \frac{1}{2} \int_{\chi}^1 \frac{dy}{y} \left[C_{1,q}(y, \xi) s\left(\frac{\chi}{y}, Q\right) + C_{1,g}(y, \xi) g\left(\frac{\chi}{y}, Q\right) \right] \quad (1.30)$$

$$F_2^H(x, Q, m_H) = \chi \int_{\chi}^1 \frac{dy}{y} \left[C_{2,q}(y, \xi) s\left(\frac{\chi}{y}, Q\right) + C_{2,g}(y, \xi) g\left(\frac{\chi}{y}, Q\right) \right] \quad (1.31)$$

$$F_3^H(x, Q, m_H) = \int_{\chi}^1 \frac{dy}{y} \left[C_{3,q}(y, \xi) s\left(\frac{\chi}{y}, Q\right) + C_{3,g}(y, \xi) g\left(\frac{\chi}{y}, Q\right) \right] \quad (1.32)$$

with:

$$\chi = x \left(1 + \frac{m_H^2}{Q^2} \right) = \frac{x}{\lambda}, \quad (1.33)$$

where:

$$\lambda = \frac{Q^2}{Q^2 + m_H^2} = \frac{\xi}{1 + \xi}. \quad (1.34)$$

Now, defining:

$$F_L^H(x, Q, m_H) = F_2^H(x, Q, m_H) - 2xF_1^H(x, Q, m_H), \quad (1.35)$$

we have that:

$$F_L^H(x, Q, m_H) = \chi \int_{\chi}^1 \frac{dy}{y} \left[C_{L,q}(y, \xi) s\left(\frac{\chi}{y}, Q\right) + C_{L,g}(y, \xi) g\left(\frac{\chi}{y}, Q\right) \right], \quad (1.36)$$

where we have defined:

$$C_{L,q(g)}(y, \xi) = C_{2,q(g)}(y, \xi) - \lambda C_{1,q(g)}(y, \xi) \quad (1.37)$$

All the coefficient functions entering the structure functions above admit a perturbative expansion that at N^N LO reads:

$$C_{k,q(g)}(y, \xi) = \sum_{n=0}^N a_s^n(Q) C_{k,q(g)}^{(n)}(y, \xi), \quad k = 1, 2, 3, L. \quad (1.38)$$

In the following we will truncate the expansion at NLO.

After the definitions above we can write down, first the LO coefficient functions. While at LO the gluon coefficient functions are all zero ($C_{k,g}^{(0)}(y, \xi) = 0$), the quark coefficient functions are:

$$\begin{aligned} C_{1,q}^{(0)}(x, \xi) &= \delta(1-x), \\ C_{2,q}^{(0)}(x, \xi) &= \delta(1-x), \\ C_{3,q}^{(0)}(x, \xi) &= \delta(1-x), \\ C_{L,q}^{(0)}(x, \xi) &= (1-\lambda)\delta(1-x). \end{aligned} \quad (1.39)$$

The NLO charged-current massive coefficient have been computed and reported in Appendix A of Ref. [5]. However, before being implemented in APFEL they need some manipulation. We start defining:

$$K_A = \frac{1}{\lambda}(1-\lambda)\ln(1-\lambda). \quad (1.40)$$

In addition, in order to consider factorization scale variations, we also need to consider the splitting function:

$$P_{qq}^{(0)}(z) = C_F \left[\frac{1+z^2}{(1-z)_+} + \frac{3}{2}\delta(1-z) \right] = C_F \left[\frac{2}{(1-z)_+} - (1+z) + \frac{3}{2}\delta(1-z) \right], \quad (1.41)$$

and we also define:

$$K_F^2 = \frac{Q^2}{\mu_F^2}. \quad (1.42)$$

The explicit expressions of the NLO quark coefficient functions read:

$$\begin{aligned} C_{1,q}^{(1)} = & 2C_F \left\{ \left(-4 - \frac{1}{2\lambda} - 2\zeta_2 - \frac{1+3\lambda}{2\lambda}K_A + \frac{3}{2}\ln\frac{K_F^2}{\lambda} \right) \delta(1-z) \right. \\ & - \frac{(1+z^2)\ln z}{1-z} + \left(-\ln\frac{K_F^2}{\lambda} - 2\ln(1-z) + \ln(1-\lambda z) \right) (1+z) + (3-z) + \frac{1}{\lambda^2} + \frac{z-1}{\lambda} \\ & + 2 \left[\frac{2\ln(1-z) - \ln(1-\lambda z)}{1-z} \right]_+ + 2 \left(-1 + \ln\frac{K_F^2}{\lambda} \right) \left[\frac{1}{1-z} \right]_+ \\ & \left. + \frac{\lambda-1}{\lambda^2} \left[\frac{1}{1-\lambda z} \right]_+ + \frac{1}{2} \left[\frac{1-z}{(1-\lambda z)^2} \right]_+ \right\}, \quad (1.43) \end{aligned}$$

$$\begin{aligned} C_{2,q}^{(1)} = & 2C_F \left\{ \left(-4 - \frac{1}{2\lambda} - 2\zeta_2 - \frac{1+\lambda}{2\lambda}K_A + \frac{3}{2}\ln\frac{K_F^2}{\lambda} \right) \delta(1-z) \right. \\ & - \frac{(1+z^2)\ln z}{1-z} + \left(2 - \ln\frac{K_F^2}{\lambda} - 2\ln(1-z) + \ln(1-\lambda z) \right) (1+z) + \frac{1}{\lambda} \\ & + 2 \left[\frac{2\ln(1-z) - \ln(1-\lambda z)}{1-z} \right]_+ + 2 \left(-1 + \ln\frac{K_F^2}{\lambda} \right) \left[\frac{1}{1-z} \right]_+ \\ & \left. + \frac{2\lambda^2 - \lambda - 1}{\lambda} \left[\frac{1}{1-\lambda z} \right]_+ + \frac{1}{2} \left[\frac{1-z}{(1-\lambda z)^2} \right]_+ \right\}, \quad (1.44) \end{aligned}$$

$$\begin{aligned} C_{3,q}^{(1)} = & 2C_F \left\{ \left(-4 - \frac{1}{2\lambda} - 2\zeta_2 - \frac{1+3\lambda}{2\lambda}K_A + \frac{3}{2}\ln\frac{K_F^2}{\lambda} \right) \delta(1-z) \right. \\ & - \frac{(1+z^2)\ln z}{1-z} + \left(1 - \ln\frac{K_F^2}{\lambda} - 2\ln(1-z) + \ln(1-\lambda z) \right) (1+z) + \frac{1}{\lambda} \\ & + 2 \left[\frac{2\ln(1-z) - \ln(1-\lambda z)}{1-z} \right]_+ + 2 \left(-1 + \ln\frac{K_F^2}{\lambda} \right) \left[\frac{1}{1-z} \right]_+ \\ & \left. + \frac{\lambda-1}{\lambda} \left[\frac{1}{1-\lambda z} \right]_+ + \frac{1}{2} \left[\frac{1-z}{(1-\lambda z)^2} \right]_+ \right\}, \quad (1.45) \end{aligned}$$

$$\begin{aligned}
C_{L,q}^{(1)} = & 2C_F(1-\lambda) \left\{ \left(-4 - \frac{1}{2\lambda} - 2\zeta_2 - \frac{1+\lambda}{2\lambda} K_A + \frac{3}{2} \ln \frac{K_F^2}{\lambda} \right) \delta(1-z) \right. \\
& - \frac{(1+z^2) \ln z}{1-z} + \left(-\ln \frac{K_F^2}{\lambda} - 2 \ln(1-z) + \ln(1-\lambda z) \right) (1+z) + 3 \\
& + 2 \left[\frac{2 \ln(1-z) - \ln(1-\lambda z)}{1-z} \right]_+ + 2 \left(-1 + \ln \frac{K_F^2}{\lambda} \right) \left[\frac{1}{1-z} \right]_+ \\
& \left. - 2 \left[\frac{1}{1-\lambda z} \right]_+ + \frac{1}{2} \left[\frac{1-z}{(1-\lambda z)^2} \right]_+ \right\} + 2C_F [\lambda K_A \delta(1-z) + (1+\lambda)z]
\end{aligned} \tag{1.46}$$

In order to proceed with our manipulations we need to define the generalized or incomplete $+$ -prescription:

$$\int_x^1 dz [f(z)]_+ g(z) = \int_x^1 dz f(z) [g(z) - g(1)] - g(1) \underbrace{\int_0^x dz f(z)}_{-R_f(x)} \tag{1.47}$$

$$\int_x^1 dz \{ [f(z)]_+ + R_f(x) \delta(1-z) \} g(z).$$

where the $+$ -prescription in the r.h.s of the equation above should be understood in the usual way independently of the integration bounds.

Often the residual $R_f(x)$ function can be evaluated analytically by performing the integral, however sometimes it need to be evaluated numerically performing the integral in a numerical way. In particular the $+$ -prescribed functions that enter the expressions above give rise to the following residual functions that can be computed analytically:

$$-\int_0^x \frac{dz}{1-z} = \ln(1-x), \tag{1.48}$$

$$-\int_0^x dz \frac{\ln(1-z)}{1-z} = \frac{1}{2} \ln^2(1-x), \tag{1.49}$$

$$-\int_0^x \frac{dz}{1-\lambda z} = \frac{1}{\lambda} \ln(1-\lambda x), \tag{1.50}$$

$$-\int_0^x dz \frac{1-z}{(1-\lambda z)^2} = \frac{1}{\lambda^2} \ln(1-\lambda x) + \frac{1-\lambda}{\lambda} \frac{x}{1-\lambda x}, \tag{1.51}$$

while we do not know how to solve analytically the integral:

$$R(x) = -\int_0^x dz \frac{\ln(1-\lambda z)}{1-z} \tag{1.52}$$

therefore we will compute it numerically.

As a consequence, when convoluting the coefficient functions above with PDFs in the point x , we can treat the $+$ -prescribed functions using the standard definition at the price of adding to the local terms the following functions:

$$\begin{aligned}
C_{1,q}^{(1)} \rightarrow & C_{1,q}^{(1)} + 2C_F \left[2 \ln^2(1-x) - 2R(x) + 2 \left(-1 + \ln \frac{K_F^2}{\lambda} \right) \ln(1-x) \right. \\
& \left. + \frac{\lambda-1}{\lambda^3} \ln(1-\lambda x) + \frac{1}{2\lambda^2} \ln(1-\lambda x) + \frac{1-\lambda}{2\lambda} \frac{x}{1-\lambda x} \right] \delta(1-z)
\end{aligned} \tag{1.53}$$

$$\begin{aligned}
C_{2,q}^{(1)} \rightarrow & C_{2,q}^{(1)} + 2C_F \left[2 \ln^2(1-x) - 2R(x) + 2 \left(-1 + \ln \frac{K_F^2}{\lambda} \right) \ln(1-x) \right. \\
& \left. + \frac{2\lambda^2 - \lambda - 1}{\lambda^2} \ln(1-\lambda x) + \frac{1}{2\lambda^2} \ln(1-\lambda x) + \frac{1-\lambda}{2\lambda} \frac{x}{1-\lambda x} \right] \delta(1-z)
\end{aligned} \tag{1.54}$$

$$C_{3,q}^{(1)} \rightarrow C_{3,q}^{(1)} + 2C_F \left[2\ln^2(1-x) - 2R(x) + 2 \left(-1 + \ln \frac{K_F^2}{\lambda} \right) \ln(1-x) \right. \\ \left. + \frac{\lambda-1}{\lambda^2} \ln(1-\lambda x) + \frac{1}{2\lambda^2} \ln(1-\lambda x) + \frac{1-\lambda}{2\lambda} \frac{x}{1-\lambda x} \right] \delta(1-z) , \quad (1.55)$$

$$C_{L,q}^{(1)} \rightarrow C_{L,q}^{(1)} + 2C_F(1-\lambda) \left[2\ln^2(1-x) - 2R(x) + 2 \left(-1 + \ln \frac{K_F^2}{\lambda} \right) \ln(1-x) \right. \\ \left. - \frac{2}{\lambda} \ln(1-\lambda x) + \frac{1}{2\lambda^2} \ln(1-\lambda x) + \frac{1-\lambda}{2\lambda} \frac{x}{1-\lambda x} \right] \delta(1-z) . \quad (1.56)$$

Now let us consider the gluon coefficient functions, that read:

$$C_{1,g}^{(1)} = 2T_R \left\{ [z^2 + (1-z)^2] \left[\ln \left(\frac{1-z}{z} \right) - \frac{1}{2} \ln(1-\lambda) + \frac{1}{2} \ln \frac{K_F^2}{\lambda} \right] + \right. \\ \left. 4z(1-z) - 1 + (1-\lambda) \left[-4z(1-z) + \frac{z}{1-\lambda z} + 2z(1-2\lambda z) \ln \frac{1-\lambda z}{(1-\lambda)z} \right] \right\} , \quad (1.57)$$

$$C_{2,g}^{(1)} = 2T_R \left\{ [z^2 + (1-z)^2] \left[\ln \left(\frac{1-z}{z} \right) - \frac{1}{2} \ln(1-\lambda) + \frac{1}{2} \ln \frac{K_F^2}{\lambda} \right] + \right. \\ \left. 8z(1-z) - 1 + (1-\lambda) \left[-6(1+2\lambda)z(1-z) + \frac{1}{1-\lambda z} + 6\lambda z(1-2\lambda z) \ln \frac{1-\lambda z}{(1-\lambda)z} \right] \right\} , \quad (1.58)$$

$$C_{3,g}^{(1)} = 2T_R \left\{ [z^2 + (1-z)^2] \left[2\ln \left(\frac{1-z}{1-\lambda z} \right) + \frac{1}{2} \ln(1-\lambda) + \frac{1}{2} \ln \frac{K_F^2}{\lambda} \right] + \right. \\ \left. (1-\lambda) \left[2z(1-z) - 2z[1 - (1+\lambda)z] \ln \frac{1-\lambda z}{(1-\lambda)z} \right] \right\} , \quad (1.59)$$

$$C_{L,g}^{(1)} = 2T_R \left\{ (1-\lambda)[z^2 + (1-z)^2] \left[\ln \left(\frac{1-z}{z} \right) - \frac{1}{2} \ln(1-\lambda) + \frac{1}{2} \ln \frac{K_F^2}{\lambda} \right] + \right. \\ \left. 4(2-\lambda)z(1-z) + (1-\lambda) \left[-2(3+4\lambda)z(1-z) + 4\lambda z(1-2\lambda z) \ln \frac{1-\lambda z}{(1-\lambda)z} \right] \right\} . \quad (1.60)$$

Since these functions do not contain any +-prescribed functions, they can be implemented as they are.

We now consider the massless limit of the above massive coefficient functions. We start considering that:

$$\lambda \rightarrow 1 \\ K_A \rightarrow 0 , \quad (1.61)$$

as consequence we find that the quark coefficient functions tend to:

$$C_{1,q}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{1,q}^{0,(1)} = 2C_F \left\{ - \left(\frac{9}{2} + 2\zeta_2 - \frac{3}{2} \ln K_F^2 \right) \delta(1-z) \right. \\ - \frac{(1+z^2) \ln z}{1-z} - (\ln(1-z) + \ln K_F^2) (1+z) + 3 \\ \left. + 2 \left[\frac{\ln(1-z)}{1-z} \right]_+ - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \left[\frac{1}{1-z} \right]_+ \right\} \quad (1.62)$$

$$\begin{aligned}
C_{2,q}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{2,q}^{0,(1)} &= 2C_F \left\{ - \left(\frac{9}{2} + 2\zeta_2 - \frac{3}{2} \ln K_F^2 \right) \delta(1-z) \right. \\
&\quad - \frac{(1+z^2) \ln z}{1-z} - (\ln(1-z) + \ln K_F^2) (1+z) + 2z + 3 \\
&\quad \left. + 2 \left[\frac{\ln(1-z)}{1-z} \right]_+ - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \left[\frac{1}{1-z} \right]_+ \right\}
\end{aligned} \tag{1.63}$$

$$\begin{aligned}
C_{3,q}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{3,q}^{0,(1)} &= 2C_F \left\{ - \left(\frac{9}{2} + 2\zeta_2 - \frac{3}{2} \ln K_F^2 \right) \delta(1-z) \right. \\
&\quad - \frac{(1+z^2) \ln z}{1-z} - (\ln(1-z) + \ln K_F^2) (1+z) + z + 2 \\
&\quad \left. + 2 \left[\frac{\ln(1-z)}{1-z} \right]_+ - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \left[\frac{1}{1-z} \right]_+ \right\}
\end{aligned} \tag{1.64}$$

$$C_{L,q}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{L,q}^{0,(1)} = 4C_F z \tag{1.65}$$

The local term to be added to the quark coefficient functions, considering that:

$$R(x) \xrightarrow{m_H \rightarrow 0} \frac{1}{2} \ln(1-x)^2, \tag{1.66}$$

are:

$$C_{1,q}^{0,(1)} \rightarrow C_{1,q}^{0,(1)} + 2C_F \left[\ln^2(1-x) - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \ln(1-x) \right] \delta(1-z), \tag{1.67}$$

$$C_{2,q}^{0,(1)} \rightarrow C_{2,q}^{0,(1)} + 2C_F \left[\ln^2(1-x) - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \ln(1-x) \right] \delta(1-z), \tag{1.68}$$

$$C_{3,q}^{0,(1)} \rightarrow C_{3,q}^{0,(1)} + 2C_F \left[\ln^2(1-x) - \left(\frac{3}{2} - 2 \ln K_F^2 \right) \ln(1-x) \right] \delta(1-z), \tag{1.69}$$

while no local term needs to be added to $C_{L,q}^{0,(1)}$.

Now we turn to the gluon coefficient functions where we need to know that:

$$\ln(1-\lambda) \xrightarrow{m_H \rightarrow 0} -\ln \left(\frac{Q^2}{m_H^2} \right) \tag{1.70}$$

so that:

$$C_{1,g}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{1,g}^{0,(1)} = 2T_R \left\{ [z^2 + (1-z)^2] \left[\ln \left(\frac{1-z}{z} \right) + \frac{1}{2} \ln \left(\frac{Q^2}{m_H^2} \right) + \frac{1}{2} \ln K_F^2 \right] + 4z(1-z) - 1 \right\}, \tag{1.71}$$

$$C_{2,g}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{2,g}^{0,(1)} = 2T_R \left\{ [z^2 + (1-z)^2] \left[\ln \left(\frac{1-z}{z} \right) + \frac{1}{2} \ln \left(\frac{Q^2}{m_H^2} \right) + \frac{1}{2} \ln K_F^2 \right] + 8z(1-z) - 1 \right\}, \tag{1.72}$$

$$C_{3,g}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{3,g}^{0,(1)} = 2T_R [z^2 + (1-z)^2] \left[-\frac{1}{2} \ln \left(\frac{Q^2}{m_H^2} \right) + \frac{1}{2} \ln K_F^2 \right], \tag{1.73}$$

$$C_{L,g}^{(1)} \xrightarrow{m_H \rightarrow 0} C_{L,g}^{0,(1)} = 2T_R [4z(1-z)]. \tag{1.74}$$

We also note that in the limit $m_H \rightarrow 0$, the convolution integrals in eqs. (1.30), (1.31), (1.32) and (1.36) will extend from x to 1 rather than from χ to 1.

As clear from the definitions in eqs. (1.30), (1.31), (1.32) and (1.36), in order to compute a give structure functions for some given value of x , one needs to convolute the coefficient functions that we have written above with PDFs in the rescaled point $\chi = x/\lambda > x$, so in particular the convolution integral extends from χ to 1. This is a kinematical consequence of the mass of the heavy quark involved that reduces the phase space available for the process.

From the point of view of the implementation of the FONLL scheme in APFEL, given that the massive scheme needs to be combined with the massless and the massive-zero schemes whose convolution integrals

extend from x to 1, it would be convenient to rewrite eqs. (1.30), (1.31), (1.32) and (1.36) in such a way that the lower integration bound is x rather than χ . To this end, let us consider the integral:

$$I = \int_{\chi}^1 \frac{dy}{y} C(y) f\left(\frac{\chi}{y}\right), \quad (1.75)$$

where $\chi = x/\lambda$. By the change of integration variable $z = \lambda y$, we can rewrite the integral above as:

$$I = \int_x^{\lambda} \frac{dz}{z} C\left(\frac{z}{\lambda}\right) f\left(\frac{x}{y}\right) = \int_x^1 \frac{dz}{z} \tilde{C}(z, \lambda) f\left(\frac{x}{y}\right), \quad (1.76)$$

where:

$$\tilde{C}(z, \lambda) = \theta(\lambda - z) C\left(\frac{z}{\lambda}\right). \quad (1.77)$$

In this way we have achieved the goal of expressing the “reduced” convolution in eqs. (1.30), (1.31), (1.32) and (1.36) as a “standard” convolution between x and 1. The price to pay is to consider the massive coefficient functions during the integration as explicit functions of the variable z/λ and to cut off the region $z > \lambda$ by means of the Heaviside θ -function. Of course, this does not need to be done in the massive-zero case as the convolution already extends between x and 1.

2 Target Mass Corrections

Kinematic corrections due to the finite mass of the target proton M_p which recoils against the photon might be relevant in the small-energy region. The leading contributions to such corrections have been computed long time ago in Ref. [6] and, denoting the target-mass corrected structure functions with $\tilde{}$, they take the form:

$$\begin{aligned} \tilde{F}_2(x, Q) &= \frac{x^2}{\xi^2 \tau^{3/2}} F_2(\xi, Q) + \frac{6\rho x^3}{\tau^2} I_2(\xi, Q), \\ \tilde{F}_L(x, Q) &= F_L(\xi, Q) + \frac{x^2(1-\tau)}{\xi^2 \tau^{3/2}} F_2(\xi, Q) + \frac{\rho x^3(6-2\tau)}{\tau^2} I_2(\xi, Q), \\ x\tilde{F}_3(x, Q) &= \frac{x^2}{\xi^2 \tau} \xi F_3(\xi, Q) + \frac{4\rho x^3}{\tau^{3/2}} I_3(\xi, Q), \end{aligned} \quad (2.1)$$

where:

$$\rho = \frac{M_p^2}{Q^2}, \quad \tau = 1 + 4\rho x^2, \quad \xi = \frac{2x}{1 + \sqrt{\tau}}, \quad (2.2)$$

and:

$$I_2(\xi, Q) = \int_{\xi}^1 dy \frac{F_2(y, Q)}{y^2}, \quad I_3(\xi, Q) = \int_{\xi}^1 dy \frac{y F_3(y, Q)}{y^2}. \quad (2.3)$$

Using the interpolation formula, we have that:

$$\frac{F_2(y, Q)}{y^2} = \sum_{\alpha} \frac{F_2(x_{\alpha}, Q)}{x_{\alpha}^2} w_{\alpha}^{(k)}(y), \quad (2.4)$$

therefore:

$$I_2(\xi, Q) = \sum_{\alpha} \frac{F_2(x_{\alpha}, Q)}{x_{\alpha}^2} \int_{\xi}^1 dy w_{\alpha}^{(k)}(y), \quad (2.5)$$

while:

$$I_3(\xi, Q) = \sum_{\alpha} \frac{x_{\alpha} F_3(x_{\alpha}, Q)}{x_{\alpha}^2} \int_{\xi}^1 dy w_{\alpha}^{(k)}(y). \quad (2.6)$$

In turn, again using the interpolation formula, we can write:

$$J_{\alpha}(\xi) \equiv \int_{\xi}^1 dy w_{\alpha}^{(k)}(y) = \sum_{\beta=0}^{N_x} \underbrace{\left[\int_{x_{\beta}}^1 dy w_{\alpha}^{(k)}(y) \right]}_{J_{\beta\alpha}} w_{\beta}^{(k)}(\xi). \quad (2.7)$$

Considering the fact that:

$$w_\alpha^{(k)}(y) \neq 0 \quad \text{for} \quad x_{\alpha-k} < y < x_{\alpha+1}, \quad (2.8)$$

it follows that:

$$J_{\beta\alpha} = 0 \quad \text{for} \quad \beta > \alpha \quad (2.9)$$

and thus:

$$J_\alpha(\xi) = \sum_{\beta=0}^{\alpha} J_{\beta\alpha} w_\beta^{(k)}(\xi). \quad (2.10)$$

In addition, we can simplify the integral as follows:

$$J_{\beta\alpha} = \int_c^d dy w_\alpha^{(k)}(y), \quad (2.11)$$

where:

$$c = \max(x_\beta, x_{\alpha-k}) \quad \text{and} \quad d = \min(1, x_{\alpha+1}). \quad (2.12)$$

In conclusion, we can treat $J_{\beta\alpha}$ exactly in the same manner as the regular part of a massless coefficient function or a splitting function and thus it can be precomputed and stored.

At the end of the day we have that:

$$I_2(\xi, Q) = \sum_{\alpha=0}^{N_x} \sum_{\beta=0}^{\alpha} w_\beta^{(k)}(\xi) J_{\beta\alpha} \frac{F_2(x_\alpha, Q)}{x_\alpha^2}, \quad (2.13)$$

that can also be written as:

$$I_2(\xi, Q) = \sum_{\beta=0}^{N_x} \underbrace{\left[\sum_{\alpha=\beta}^{N_x} J_{\beta\alpha} \frac{F_2(x_\alpha, Q)}{x_\alpha^2} \right]}_{I_2(x_\beta, Q)} w_\beta^{(k)}(\xi). \quad (2.14)$$

Similarly:

$$I_3(\xi, Q) = \sum_{\beta=0}^{N_x} \underbrace{\left[\sum_{\alpha=\beta}^{N_x} J_{\beta\alpha} \frac{x_\alpha F_3(x_\alpha, Q)}{x_\alpha^2} \right]}_{I_3(x_\beta, Q)} w_\beta^{(k)}(\xi). \quad (2.15)$$

Gathering all pieces we finally find:

$$\begin{aligned} \tilde{F}_2(x, Q) &= \sum_{\beta=0}^{N_x} \left[\frac{x^2}{\xi^2 \tau^{3/2}} F_2(x_\beta, Q) + \frac{6\rho x^3}{\tau^2} I_2(x_\beta, Q) \right] w_\beta^{(k)}(\xi), \\ \tilde{F}_L(x, Q) &= \sum_{\beta=0}^{N_x} \left[F_L(x_\beta, Q) + \frac{x^2(1-\tau)}{\xi^2 \tau^{3/2}} F_2(x_\beta, Q) + \frac{\rho x^3(6-2\tau)}{\tau^2} I_2(x_\beta, Q) \right] w_\beta^{(k)}(\xi), \\ x\tilde{F}_3(x, Q) &= \sum_{\beta=0}^{N_x} \left[\frac{x^2}{\xi^2 \tau} x_\beta F_3(x_\beta, Q) + \frac{4\rho x^3}{\tau^{3/2}} I_3(x_\beta, Q) \right] w_\beta^{(k)}(\xi). \end{aligned} \quad (2.16)$$

For the equations above is clear that in the case when $M_p = 0$, that implies $\rho = 0$, $\tau = 1$ and $\xi = x$, all structure functions reduce to the uncorrected formulas.

When considering the extraction of the DIS operator times the evolution operator like in eq. (1.15), one should be careful with I_2 and I_3 . Considering that:

$$F(x_\alpha, Q) = \sum_{\gamma, \delta} \sum_{i, j} \Gamma_{i, \alpha\gamma}(Q) M_{ij, \gamma\delta}(Q, Q_0) \tilde{q}_j(x_\delta, Q_0) \quad (2.17)$$

we have that:

$$I(x_\beta, Q) = \sum_{\alpha=\beta}^{N_x} J_{\beta\alpha} \frac{F(x_\alpha, Q)}{x_\alpha^2} = \sum_{\gamma, \delta} \sum_{i, j} \left[\sum_{\alpha=\beta}^{N_x} \frac{J_{\beta\alpha} \Gamma_{i, \alpha\gamma}(Q)}{x_\alpha^2} \right] M_{ij, \gamma\delta}(Q, Q_0) \tilde{q}_j(x_\delta, Q_0), \quad (2.18)$$

3 Renormalization and Factorization Scale Variation

In the previous sections, when discussing the implementation of the structure functions in APFEL, we assumed that the renormalization scale μ_R and the factorization scale μ_F were identified to the scale of the process Q . In this section, we want to relax this assumption and to do so we the expansion of the DGLAP and RG equation for α_s up to NLO, that is:

$$\frac{\partial f_i}{\partial \ln \mu_F^2} = \frac{\alpha_s(\mu_F)}{4\pi} \left[P_{ij}^{(0)}(x) + \frac{\alpha_s(\mu_F)}{4\pi} P_{ij}^{(1)}(x) + \dots \right] \otimes f_j(x, \mu_F), \quad (3.1)$$

and:

$$\frac{\partial}{\partial \ln \mu_R^2} \left(\frac{\alpha_s}{4\pi} \right) = - \left(\frac{\alpha_s(\mu_R)}{4\pi} \right)^2 \left[\beta_0 + \frac{\alpha_s(\mu_R)}{4\pi} \beta_1 + \dots \right]. \quad (3.2)$$

Defining:

$$\xi_R \equiv \frac{\mu_R}{Q}, \quad \xi_F \equiv \frac{\mu_F}{Q} \quad \text{and} \quad a_s = \frac{\alpha_s}{4\pi} \quad (3.3)$$

where Q is constant, and defining:

$$t_R \equiv \ln \xi_R^2 \quad \text{and} \quad t_F \equiv \ln \xi_F^2, \quad (3.4)$$

the equations above can be written as:

$$\frac{\partial f_i}{\partial t_F} = a_s(t_F) \left[P_{ij}^{(0)} + a_s(t_F) P_{ij}^{(1)} + \dots \right] \otimes f_j(t_F), \quad (3.5)$$

and:

$$\frac{\partial a_s}{\partial t_R} = -a_s^2(t_R) [\beta_0 + a_s(t_R) \beta_1 + \dots]. \quad (3.6)$$

Now, expanding $f_i(t)$ around $t = t_F$ we have:

$$f_i(t) = f_i(t_F) + \frac{\partial f_i}{\partial t} \Big|_{t=t_F} (t - t_F) + \frac{1}{2} \frac{\partial^2 f_i}{\partial t^2} \Big|_{t=t_F} (t - t_F)^2 + \dots \quad (3.7)$$

Using eqs. (3.5) and (3.6), we have that:

$$\begin{aligned} \frac{\partial f_i}{\partial t} \Big|_{t=t_F} &= \left[a_s(t_F) P_{ij}^{(0)} + a_s^2(t_F) P_{ij}^{(1)} \right] \otimes f_j(t_F) + \mathcal{O}(a_s^3) \\ \frac{\partial^2 f_i}{\partial t^2} \Big|_{t=t_F} &= a_s^2(t_F) \left[P_{il}^{(0)} \otimes P_{lj}^{(0)} - \beta_0 P_{ij}^{(0)} \right] \otimes f_j(t_F) + \mathcal{O}(a_s^3) \end{aligned} \quad (3.8)$$

Choosing $t = 0$ in eq. (3.7), we finally have:

$$f_i(0) = \left\{ 1 - a_s(t_F) t_F P_{ij}^{(0)} + a_s^2(t_F) \left[-t_F P_{ij}^{(1)} + t_F^2 \frac{1}{2} \left(P_{il}^{(0)} \otimes P_{lj}^{(0)} - \beta_0 P_{ij}^{(0)} \right) \right] \right\} \otimes f_j(t_F) + \mathcal{O}(a_s^3). \quad (3.9)$$

Now, using eq. (3.6), we easily find:

$$a_s(t_F) = a_s(t_R) \left[1 + a_s(t_R) \beta_0 (t_R - t_F) + \mathcal{O}(a_s^2) \right], \quad (3.10)$$

which can be plugged into eq. (3.9) to give:

$$f_i(0) = \left\{ 1 - a_s(t_R) t_F P_{ij}^{(0)} + a_s^2(t_R) \left[-t_F P_{ij}^{(1)} + t_F^2 \frac{1}{2} \left(P_{il}^{(0)} \otimes P_{lj}^{(0)} + \beta_0 P_{ij}^{(0)} \right) - t_F t_R \beta_0 P_{ij}^{(0)} \right] \right\} \otimes f_j(t_F) + \mathcal{O}(a_s^3). \quad (3.11)$$

Finally, setting $t_F = 0$ in eq. (3.10), we find:

$$a_s(0) = a_s(t_R) \left[1 + a_s(t_R) \beta_0 t_R + \mathcal{O}(a_s^2) \right], \quad (3.12)$$

Considering that and NNLO the ZM structure functions are written in terms of PDFs and coefficient functions as:

$$F(t_R, t_F)/x = \left[\sum_{k=0}^2 a_s^k(t_R) \tilde{\mathcal{C}}_i^{(k)}(t_R, t_F) \right] \otimes f_i(t_F) + \mathcal{O}(a_s^3), \quad (3.13)$$

and that, up to subleading terms, the structure functions must be renormalization and factorization scale independent, this requires that:

$$F(t_R, t_F) = F(0, 0). \quad (3.14)$$

But since:

$$F(0, 0)/x = \left[\sum_{k=0}^2 a_s^k(0) \tilde{C}_i^{(k)} \right] \otimes f_i(0) + \mathcal{O}(a_s^3), \quad (3.15)$$

where $\tilde{C}_i^{(k)}$ are the well-know ZM coefficient functions, using eqs. (3.11) and (3.12) in eq. (3.15) and finally imposing the identity in eq. (3.14), we can find the explicit expression of the “generalized” coefficient functions $\tilde{C}_i^{(k)}(t_R, t_F)$. In fact:

$$\begin{aligned} F(0, 0)/x &= \left\{ \tilde{C}_j^{(0)} \right. \\ &+ a_s(t_R) \left[\tilde{C}_j^{(1)} - t_F \tilde{C}_i^{(0)} \otimes P_{ij}^{(0)} \right] \\ &+ a_s^2(t_R) \left[\tilde{C}_j^{(2)} + t_R \beta_0 \tilde{C}_j^{(1)} - t_F \left(\tilde{C}_i^{(0)} \otimes P_{ij}^{(1)} + \tilde{C}_i^{(1)} \otimes P_{ij}^{(0)} \right) \right. \\ &\left. \left. + \frac{t_F^2}{2} \tilde{C}_i^{(0)} \otimes \left(P_{il}^{(0)} \otimes P_{lj}^{(0)} + \beta_0 P_{ij}^{(0)} \right) - t_F t_R \beta_0 \tilde{C}_i^{(0)} \otimes P_{ij}^{(0)} \right] \right\} \otimes f_j(t_F) + \mathcal{O}(a_s^3). \end{aligned} \quad (3.16)$$

Finally, using the identity in eq. (3.14), it is easy to find that:

$$\begin{aligned} \tilde{C}_j^{(0)}(t_R, t_F) &= \tilde{C}_j^{(0)} \\ \tilde{C}_j^{(1)}(t_R, t_F) &= \tilde{C}_j^{(1)} - t_F \tilde{C}_i^{(0)} \otimes P_{ij}^{(0)} \\ \tilde{C}_j^{(2)}(t_R, t_F) &= \tilde{C}_j^{(2)} + t_R \beta_0 \tilde{C}_j^{(1)} - t_F \left(\tilde{C}_i^{(0)} \otimes P_{ij}^{(1)} + \tilde{C}_i^{(1)} \otimes P_{ij}^{(0)} \right) \\ &+ \frac{t_F^2}{2} \tilde{C}_i^{(0)} \otimes \left(P_{il}^{(0)} \otimes P_{lj}^{(0)} + \beta_0 P_{ij}^{(0)} \right) - t_F t_R \beta_0 \tilde{C}_i^{(0)} \otimes P_{ij}^{(0)}. \end{aligned} \quad (3.17)$$

Therefore, in the ZM-VFNS, in order to perform scale variation we need to precompute the additional convolutions: $\tilde{C}_i^{(0)} \otimes P_{ij}^{(0)}$, $\tilde{C}_i^{(0)} \otimes P_{ij}^{(1)}$, $\tilde{C}_i^{(1)} \otimes P_{ij}^{(0)}$ and $\tilde{C}_i^{(0)} \otimes P_{il}^{(0)} \otimes P_{lj}^{(0)}$.

In order to proceed, it is opportune to specify the basis in which PDFs are expressed. As usual, the most natural choice is the QCD evolution basis $\{\Sigma, g, V, V_3, V_8, V_{15}, V_{24}, V_{35}, T_3, T_8, V_{15}, T_{24}, T_{35}\}$ and thus the indices i, j and l in eq. (3.17) run between 1 and 13 over this basis. The advantage of this basis is the fact that the splitting function matrix P_{ij} is almost completely diagonalized. The starting point, is the usual definition that, up to a factor x and omitting the convolution symbol \otimes , can be written as:

$$F = \langle e_q^2 \rangle \left\{ C_g g + \sum_{i=u}^t \underbrace{\theta(Q^2 - m_i^2) \left[C_{PS} + \frac{e_i^2}{\langle e_q^2 \rangle} C_+ \right]}_{\tilde{C}_i} q_i^+ \right\}, \quad (3.18)$$

where:

$$\langle e_q^2 \rangle = \sum_{i=u}^t e_i^2 \theta(Q^2 - m_i^2). \quad (3.19)$$

Now, in order to express the structure function in eq. (3.18) in the evolution basis, we need to find the tranformation such that:

$$q_i^+ = \sum_{j=1}^6 T_{ij} f_j, \quad (3.20)$$

where f_j belongs to the evolution basis, that is: $f_1 = \Sigma$, $f_2 = T_3$, $f_3 = T_8$ and so on. One can show that the transformation matrix T_{ij} can be written as:

$$\begin{aligned} T_{ij} &= \theta(j-i) \frac{1-\delta_{ij}j}{j(j-1)} \quad j \geq 2, \\ T_{i1} &= \frac{1}{6}, \end{aligned} \quad (3.21)$$

with $\theta(j-i) = 1$ for $j \geq i$ and zero otherwise. In addition, one can show that:

$$\sum_{j=1}^6 T_{ij} = 0, \quad \text{and} \quad \sum_{i=1}^6 T_{ij} = \delta_{1j}. \quad (3.22)$$

Now, we can plug eq. (3.20) into eq. (3.18) and, using eq. (3.21), we get:

$$F = \langle e_q^2 \rangle \left\{ C_g g + \frac{1}{6} (C_+ + n_f C_{\text{PS}}) \Sigma + \sum_{j=2}^6 \frac{1}{j(j-1)} \left[\sum_{i=1}^j \hat{C}_i - j \hat{C}_j \right] f_j \right\}, \quad (3.23)$$

where we have transmuted the sum over u, d and so on into a sum between 1 and 6 and where we have defined:

$$n_f = \sum_{i=1}^6 \theta(Q^2 - m_i^2). \quad (3.24)$$

Now we need to express the term in square brackets in terms of the usual coefficient functions C_+ and C_{PS} , in particular:

$$\sum_{i=1}^j \hat{C}_i - j \hat{C}_j = \sum_{i=1}^j \theta(Q^2 - m_i^2) \left(C_{\text{PS}} + \frac{e_i^2}{\langle e_q^2 \rangle} C_+ \right) - j \theta(Q^2 - m_j^2) \left(C_{\text{PS}} + \frac{e_j^2}{\langle e_q^2 \rangle} C_+ \right). \quad (3.25)$$

Here we can distinguish two cases, the first is $Q^2 < m_j^2$ and under this assumption we have:

$$\sum_{i=1}^j \hat{C}_i - j \hat{C}_j = C_+ + n_f C_{\text{PS}}. \quad (3.26)$$

If instead $Q^2 \geq m_j^2$, then:

$$\sum_{i=1}^j \hat{C}_i - j \hat{C}_j = K_j C_+, \quad (3.27)$$

with:

$$K_j = \frac{1}{\langle e_q^2 \rangle} \left(\sum_{i=1}^j e_i^2 - j e_j^2 \right) = \frac{1}{\langle e_q^2 \rangle} \left(\sum_{i=1}^{j-1} e_i^2 - (j-1) e_j^2 \right). \quad (3.28)$$

We can express both cases in one single formula as:

$$\sum_{i=1}^j \hat{C}_i - j \hat{C}_j = \theta(m_j^2 - Q^2 - \epsilon) [C_+ + n_f C_{\text{PS}}] + \theta(Q^2 - m_j^2) [K_j C_+]. \quad (3.29)$$

where ϵ is a small parameter that ensures that the case $Q^2 = m_j^2$ is included in the second term of the r.h.s. of eq. (3.29). Eq. (3.29) can also be written as:

$$\sum_{i=1}^j \hat{C}_i - j \hat{C}_j = \theta(n_f - j) [K_j C_+] + \theta(j - n_f - 1) [C_+ + n_f C_{\text{PS}}]. \quad (3.30)$$

In addition, one can easily see that:

$$f_j = \theta(n_f - j) f_j + \theta(j - n_f - 1) \Sigma, \quad (3.31)$$

and thus:

$$\sum_{j=2}^6 \frac{1}{j(j-1)} \left[\sum_{i=1}^j \hat{C}_i - j \hat{C}_j \right] f_j = C_+ \left[\sum_{j=2}^{n_f} \frac{K_j}{j(j-1)} f_j \right] + \left[\sum_{j=n_f+1}^6 \frac{1}{j(j-1)} \right] [C_+ + n_f C_{\text{PS}}] \Sigma, \quad (3.32)$$

but:

$$\sum_{j=n_f+1}^6 \frac{1}{j(j-1)} = \frac{1}{n_f} - \frac{1}{6}, \quad (3.33)$$

Moreover:

$$\frac{K_j}{j(j-1)} = \frac{1}{\langle e_q^2 \rangle} \frac{1}{j(j-1)} \left(\sum_{i=1}^j e_i^2 - j e_j^2 \right) = \frac{1}{\langle e_q^2 \rangle} \frac{1}{j(j-1)} \underbrace{\sum_{i=1}^6 e_i^2 [\theta(j-i) - j \delta_{ij}]}_{d_j}. \quad (3.34)$$

Finally, putting all pieces together, we find:

$$F = \langle e_q^2 \rangle \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] + C_+ \sum_{j=2}^{n_f} d_j f_j. \quad (3.35)$$

It is interesting to separate the contributions coming from the different flavors. To do so, we just need to separate the contributions coming from, say the k -th charge e_k^2 and this is easily done applying the following replacement:

$$e_i^2 \rightarrow \delta_{ik} e_i^2. \quad (3.36)$$

In this way we have that:

$$\langle e_q^2 \rangle \rightarrow \theta(Q^2 - m_k^2) e_k^2, \quad (3.37)$$

and:

$$d_j \rightarrow \frac{e_k^2 [\theta(j-k) - j \delta_{kj}]}{j(j-1)} = \theta(Q^2 - m_k^2) e_k^2 \frac{[\theta(j-k) - j \delta_{kj}]}{j(j-1)}, \quad (3.38)$$

so that the k -th component of the structure function F is:

$$\begin{aligned} F^{(k)} &= \theta(Q^2 - m_k^2) e_k^2 \left\{ \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] + C_+ \sum_{j=2}^{n_f} \frac{[\theta(j-k) - j \delta_{kj}]}{j(j-1)} f_j \right\} \\ &= \theta(Q^2 - m_k^2) e_k^2 \left\{ \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] - \frac{1}{k} C_+ f_k + C_+ \sum_{j=k+1}^{n_f} \frac{1}{j(j-1)} f_j \right\} \end{aligned} \quad (3.39)$$

and it is such that:

$$F = \sum_{k=1}^6 F^{(k)}. \quad (3.40)$$

In APFEL we split the total structure functions into a light component and three heavy quark components. The light components is defined as:

$$F^l = \sum_{k=1}^3 F^{(k)} = \langle e_l^2 \rangle \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] + C_+ \sum_{j=2}^{n_f} d_j^{(l)} f_j. \quad (3.41)$$

where:

$$\langle e_l^2 \rangle = \sum_{i=1}^3 e_i^2, \quad (3.42)$$

and:

$$d_j^{(l)} = \frac{1}{j(j-1)} \sum_{i=1}^3 e_i^2 [\theta(j-i) - j \delta_{ij}] = \begin{cases} \frac{1}{2} (e_u^2 - e_d^2), & j = 2 \\ \frac{1}{6} (e_u^2 + e_d^2 - 2e_s^2), & j = 3 \\ \frac{\langle e_l^2 \rangle}{j(j-1)}, & j \geq 4 \end{cases}, \quad (3.43)$$

no need of the θ -functions as the scale Q will always be above the strange threshold. This way the explicit form of F^l is:

$$F^l = \langle e_l^2 \rangle \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] + \frac{1}{2} (e_u^2 - e_d^2) C_+ T_3 + \frac{1}{6} (e_u^2 + e_d^2 - 2e_s^2) C_+ T_8 + \langle e_l^2 \rangle C_+ \sum_{j=4}^{n_f} \frac{1}{j(j-1)} f_j. \quad (3.44)$$

The heavy-quark components are instead defined as:

$$\begin{aligned} F^c &= \theta(Q^2 - m_c^2) e_c^2 \left\{ \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] - \frac{1}{4} C_+ T_{15} + C_+ \sum_{j=5}^{n_f} \frac{1}{j(j-1)} f_j \right\}, \\ F^b &= \theta(Q^2 - m_b^2) e_b^2 \left\{ \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] - \frac{1}{5} C_+ T_{24} + C_+ \sum_{j=6}^{n_f} \frac{1}{j(j-1)} f_j \right\}, \\ F^t &= \theta(Q^2 - m_t^2) e_t^2 \left\{ \left[C_g g + \left(C_{\text{PS}} + \frac{1}{n_f} C_+ \right) \Sigma \right] - \frac{1}{6} C_+ T_{35} \right\}. \end{aligned} \quad (3.45)$$

To conclude the treatment of all the structure functions, we should add that eq. (3.35) is valid only for F_2 and F_L . However, F_3 can be easily derived following the very same steps with the only differences are that: the distributions $\{\Sigma, T_3, T_8, T_{15}, T_{24}, T_{35}\}$ must be replaced with $\{V, V_3, V_8, V_{15}, V_{24}, V_{35}\}$, C_+ must be replaced with C_- , the gluon and the pure-singlet coefficient functions are identically zero and the squared electric charges replaced with the appropriate electroweak charges c_i . Following this recipe, we find:

$$F_3 = \langle c_q^2 \rangle \frac{1}{n_f} C_- V + C_- \sum_{j=2}^{n_f} d_j g_j, \quad (3.46)$$

where g_j belongs to $\{V, V_3, V_8, V_{15}, V_{24}, V_{35}\}$.

Eq. (3.35), explicitly written in eqs. (3.44) and (3.45), is the final result that allows us to implement the scale variation formulae given in eq. (3.17) in APFEL. The good aspect of eq. (3.35) is the fact that it is written in terms of the fundamental coefficient functions C_g , C_+ and C_{PS} and PDFs appear in the evolution basis where the splitting-function matrix diagonalizes. In particular, up to $\mathcal{O}(\alpha_s^2)$, we have that:

$$\begin{aligned} P_{ij}^{(k)} &\rightarrow P_{ij}^{(k)} & i, j &= g, q(\Sigma) \\ P_{ij}^{(k)} &\rightarrow \delta_{ij} P_+^{(k)} & i, j &= T_3, T_8, V_{15}, T_{24}, T_{35} \\ P_{ij}^{(k)} &\rightarrow \delta_{ij} P_-^{(k)} & i, j &= V, V_3, V_8, V_{15}, V_{24}, V_{35} \end{aligned} \quad (3.47)$$

Also, defining:

$$C_q = C_{\text{PS}} + \frac{1}{n_f} C_+, \quad (3.48)$$

we can connect eq. (3.15) and eq. (3.35) by observing that:

$$\begin{aligned} \tilde{C}_j^{(k)} &\rightarrow \langle e_q^2 \rangle C_j^{(k)} & j &= g, q(\Sigma) \\ \tilde{C}_j^{(k)} &\rightarrow d_j C_+^{(k)} & j &= T_3, T_8, T_{15}, T_{24}, T_{35} \\ \tilde{C}_j^{(k)} &\rightarrow d_j C_-^{(k)} & j &= V_3, V_8, V_{15}, V_{24}, V_{35} \end{aligned} \quad (3.49)$$

where we have also considered the “minus” distributions that appear in the F_3 structure function. Of course, the same relations must hold also for eq. (3.13):

$$\begin{aligned} \tilde{\mathcal{C}}_j^{(k)} &\rightarrow \langle e_q^2 \rangle \mathcal{C}_j^{(k)} & j &= g, q(\Sigma) \\ \tilde{\mathcal{C}}_j^{(k)} &\rightarrow d_j \mathcal{C}_+^{(k)} & j &= T_3, T_8, T_{15}, T_{24}, T_{35} \\ \tilde{\mathcal{C}}_j^{(k)} &\rightarrow d_j \mathcal{C}_-^{(k)} & j &= V_3, V_8, V_{15}, V_{24}, V_{35} \end{aligned} \quad (3.50)$$

with

$$\mathcal{C}_q = \mathcal{C}_{\text{PS}} + \frac{1}{n_f} \mathcal{C}_+. \quad (3.51)$$

In addition, in the following, we will make use of the following identity:

$$P_-^{(0)} = P_+^{(0)} = P_{qq}^{(0)}. \quad (3.52)$$

Now, considering that C_{PS} starts at $\mathcal{O}(\alpha_s^2)$, we can write:

$$\begin{aligned} C_-^{(0)}(x) &= C_+^{(0)}(x) = \Delta_{\text{SF}} \delta(1-x) \\ C_j^{(0)}(x) &= (\Delta_{\text{SF}}/n_f) \delta_{qj} \delta(1-x) \quad \text{for } j = q, g \end{aligned} \quad (3.53)$$

where $\Delta_{\text{SF}} = 1$ for F_2 and F_3 and $\Delta_{\text{SF}} = 0$ for F_L . From eq. (3.17) it follows that:

$$\begin{aligned} \mathcal{C}_\pm^{(0)}(t_R, t_F) &= \Delta_{\text{SF}} \delta(1-x) \\ \mathcal{C}_\pm^{(1)}(t_R, t_F) &= C_\pm^{(1)} - \Delta_{\text{SF}} t_F P_{qq}^{(0)} \\ \mathcal{C}_\pm^{(2)}(t_R, t_F) &= C_\pm^{(2)} + t_R \beta_0 C_\pm^{(1)} - t_F \left(\Delta_{\text{SF}} P_\pm^{(1)} + C_\pm^{(1)} \otimes P_{qq}^{(0)} \right) \\ &\quad + \Delta_{\text{SF}} \frac{t_F^2}{2} \left(P_{qq}^{(0)} \otimes P_{qq}^{(0)} + \beta_0 P_{qq}^{(0)} \right) - \Delta_{\text{SF}} t_F t_R \beta_0 P_{qq}^{(0)}, \end{aligned} \quad (3.54)$$

that can be rearranged as:

$$\begin{aligned} \mathcal{C}_\pm^{(0)}(t_R, t_F) &= \Delta_{\text{SF}} \delta(1-x) \\ \mathcal{C}_\pm^{(1)}(t_R, t_F) &= C_\pm^{(1)} - \Delta_{\text{SF}} t_F P_{qq}^{(0)} \\ \mathcal{C}_\pm^{(2)}(t_R, t_F) &= C_\pm^{(2)} + t_R \beta_0 C_\pm^{(1)} - t_F C_\pm^{(1)} \otimes P_{qq}^{(0)} \\ &\quad + \Delta_{\text{SF}} \frac{t_F^2}{2} \left(P_{qq}^{(0)} \otimes P_{qq}^{(0)} - \beta_0 P_{qq}^{(0)} \right) - \Delta_{\text{SF}} t_F \left[P_\pm^{(1)} - (t_F - t_R) \beta_0 P_{qq}^{(0)} \right]. \end{aligned} \quad (3.55)$$

The term in square brackets in the r.h.s. of the third line corresponds to what we would call $\mathcal{P}_\pm^{(1)}(t_R, t_F)$, that is the NLO splitting function in the presence of scale variations ($\mu_R \neq \mu_F$). This quantity is already evaluated by APFEL and thus does not need to be recomputed.

Now, let us consider the singlet sector that, considering the fact that becomes:

$$\begin{aligned} \mathcal{C}_j^{(0)}(t_R, t_F) &= \frac{\Delta_{\text{SF}}}{n_f} \delta_{qj} \delta(1-x) \\ \mathcal{C}_j^{(1)}(t_R, t_F) &= C_j^{(1)} - \frac{\Delta_{\text{SF}}}{n_f} t_F P_{qj}^{(0)} \\ \mathcal{C}_j^{(2)}(t_R, t_F) &= C_j^{(2)} + t_R \beta_0 C_j^{(1)} - t_F C_i^{(1)} \otimes P_{ij}^{(0)} \\ &\quad + \frac{\Delta_{\text{SF}}}{n_f} \frac{t_F^2}{2} \left(P_{qi}^{(0)} \otimes P_{ij}^{(0)} - \beta_0 P_{qj}^{(0)} \right) - \frac{\Delta_{\text{SF}}}{n_f} t_F \tilde{P}_{qj}^{(1)}. \end{aligned} \quad (3.56)$$

for $j = g, q$. Taking into account eq. (3.55) and considering also the fact that $C_{\text{PS}}^{(0)} = C_{\text{PS}}^{(1)} = 0$ (i.e. C_{PS} is $\mathcal{O}(\alpha_s^2)$), it is easy to see that:

$$\begin{aligned} \mathcal{C}_{\text{PS}}^{(0)}(t_R, t_F) &= 0 \\ \mathcal{C}_{\text{PS}}^{(1)}(t_R, t_F) &= 0 \\ \mathcal{C}_{\text{PS}}^{(2)}(t_R, t_F) &= C_{\text{PS}}^{(2)} - t_F C_g^{(1)} \otimes P_{gq}^{(0)} + \frac{\Delta_{\text{SF}}}{n_f} \frac{t_F^2}{2} P_{qg}^{(0)} \otimes P_{gq}^{(0)} - \frac{\Delta_{\text{SF}}}{n_f} t_F \left[\tilde{P}_{qg}^{(1)} - \tilde{P}_+^{(1)} \right] \end{aligned} \quad (3.57)$$

and also that:

$$\begin{aligned}
C_g^{(0)}(t_R, t_F) &= 0 \\
C_g^{(1)}(t_R, t_F) &= C_g^{(1)} - \frac{\Delta_{\text{SF}}}{n_f} t_F P_{qg}^{(0)} \\
C_g^{(2)}(t_R, t_F) &= C_g^{(2)} + t_R \beta_0 C_g^{(1)} - t_F C_i^{(1)} \otimes P_{ig}^{(0)} \\
&\quad + \frac{\Delta_{\text{SF}}}{n_f} \frac{t_F^2}{2} \left(P_{qi}^{(0)} \otimes P_{ig}^{(0)} - \beta_0 P_{qg}^{(0)} \right) - \frac{\Delta_{\text{SF}}}{n_f} t_F \tilde{P}_{qg}^{(1)},
\end{aligned} \tag{3.58}$$

where the term $C_i^{(1)} \otimes P_{ig}^{(0)}$ in the r.h.s. of the third line of eq. (3.58) should be interpreted as:

$$C_i^{(1)} \otimes P_{ig}^{(0)} = \frac{1}{n_f} C_+^{(1)} \otimes P_{qg}^{(0)} + C_g^{(1)} \otimes P_{gg}^{(0)}. \tag{3.59}$$

Now we consider the massive scheme. In the neutral-current sector the leading-order coefficient functions $C_i^{(0)}$ are identically equal to zero and this simplifies substantially the structure of the massive coefficient functions in the presence of scale variations:

$$\begin{aligned}
C_j^{(0)}(t_R, t_F) &= 0 \\
C_j^{(1)}(t_R, t_F) &= C_j^{(1)} \\
C_j^{(2)}(t_R, t_F) &= C_j^{(2)} + t_R \beta_0 C_j^{(1)} - t_F C_i^{(1)} \otimes P_{ij}^{(0)}.
\end{aligned} \tag{3.60}$$

In addition, the factorization scale variation terms are already present in the implementation of the massive coefficient functions in APFEL. As a consequence, only the renormalization variation terms need to be implemented. This is a great facilitation because the renormalization variation terms do not require any further convolution and thus no additional terms need to be computed during the initialization phase.

As far as the massive charged-current sector is concerned, no $\mathcal{O}(a_s^2)$ are presently available and thus only the first two lines of eq. (3.17) are actually needed. Also in this case the factorization scale variation terms are already present in the implementation and again this avoids the precomputation of additional terms.

Now let us discuss how to implement in APFEL the additional terms needed to perform scale variations. The only terms that are a bit more complicated to implement are those that require a convolution between two splitting functions of between a plitting functions and a coefficient functions. More in particular, we only need to compute the terms: $P_{ij}^{(0)}(x) \otimes P_{jk}^{(0)}(x)$ and $C_i^{(1)}(x) \otimes P_{ij}^{(0)}(x)$. In pricinple, these terms could be evaluated analitically by computing the explicit convolution between the know expressions that are involved. However, it seems easier in APFEL to compute these terms numerically using the ingredients that have already been evaluated in the initialization stage. To show how to reduce these terms to known quantity, let us cosider the following convolution:

$$F(x_\alpha) = x_\alpha C(x_\alpha) \otimes Q(x_\alpha) = x_\alpha \int_{x_\alpha}^1 \frac{dy}{y} C(y) Q\left(\frac{x_\alpha}{y}\right) = \int_{x_\alpha}^1 \frac{dy}{y} y C(y) \frac{x_\alpha}{y} Q\left(\frac{x_\alpha}{y}\right) = \int_{x_\alpha}^1 \frac{dy}{y} \tilde{C}(y) \tilde{Q}\left(\frac{x_\alpha}{y}\right), \tag{3.61}$$

where x_α is node of the x -space grid of APFEL and $\tilde{C}(y) = yC(y)$ and $\tilde{Q}(y) = yQ(y)$. Now, using the well-known interpolation formula we can write:

$$\int_{x_\alpha}^1 \frac{dy}{y} \tilde{C}(y) \tilde{Q}\left(\frac{x_\alpha}{y}\right) = \sum_\beta \underbrace{\left[\int_{x_\alpha}^1 \frac{dy}{y} \tilde{C}(y) w_\beta^{(k)}\left(\frac{x_\alpha}{y}\right) \right]}_{\Gamma_{\alpha\beta}} \tilde{Q}(x_\beta), \tag{3.62}$$

where $w_\beta^{(k)}$ are the usual interpolation functions of degree k . Now suppose that in turn:

$$\tilde{Q}(x_\beta) = x_\beta P(x_\beta) \otimes f(x_\beta) = \int_{x_\beta}^1 \frac{dz}{z} \tilde{P}(z) \tilde{f}\left(\frac{x_\beta}{z}\right) = \sum_\gamma \underbrace{\left[\int_{x_\beta}^1 \frac{dz}{z} \tilde{P}(z) w_\gamma^{(k)}\left(\frac{x_\beta}{z}\right) \right]}_{\Pi_{\beta\gamma}} \tilde{f}(x_\gamma), \tag{3.63}$$

it follows that:

$$F(x_\alpha) = \tilde{C}(x_\alpha) \otimes \tilde{P}(x_\alpha) \otimes \tilde{f}(x_\alpha) = \sum_{\beta, \gamma} \Gamma_{\alpha\beta} \Pi_{\beta\gamma} \tilde{f}(x_\gamma). \quad (3.64)$$

The formula above clearly shows that the missing pieces can be easily obtained by properly multiplying the precomputed splitting function matrices $\Pi_{ij, \alpha\beta}$ and the coefficient function matrices $\Gamma_{i, \alpha\beta}$ according to the scale variation formulas derived above.

As an alternative to the numerical convolution of the new pieces arising when including renormalization- and factorization-scale variations, one can try to compute the analytically the convolutions above. In fact, all the terms involved in the new convolutions are usually simple enough to make the analytic computation possible using, for instance, Mathematica. This is advantageous because it avoids any inaccuracy of numerical origin coming from the numerical convolution of the operators involved. In order to do so, we only need to know how to treat some particular term that appear in the combinations. In particular, we need to be able to treat terms in which Dirac δ -functions and $+$ -prescribed functions are present at the same time. The most trivial convolutions are those involving one or two δ -functions, that is:

$$\begin{aligned} \delta(1-x) \otimes \delta(1-x) &= \delta(1-x), \\ \left(\frac{\ln^n(1-x)}{1-x} \right)_+ \otimes \delta(1-x) &= \left(\frac{\ln^n(1-x)}{1-x} \right)_+ \quad n \geq 0, \end{aligned} \quad (3.65)$$

that can be easily proven in Mellin space where the convolution \otimes becomes a simple product and the δ -function corresponds to the unity. The Mellin-space method can be used also in the cases where two $+$ -prescribed functions are involved. Up to $\mathcal{O}(\alpha_s^2)$ there are only two possible combinations, that are:

$$\begin{aligned} \left(\frac{1}{1-x} \right)_+ \otimes \left(\frac{1}{1-x} \right)_+ &= 2 \left(\frac{\ln(1-x)}{1-x} \right)_+ - \frac{\ln(x)}{1-x} - \zeta(2)\delta(1-x), \\ \left(\frac{1}{1-x} \right)_+ \otimes \left(\frac{\ln(1-x)}{1-x} \right)_+ &= \frac{3}{2} \left(\frac{\ln^2(1-x)}{1-x} \right)_+ - \zeta(2) \left(\frac{1}{1-x} \right)_+ - \frac{\ln(x) \ln(1-x)}{1-x} + \zeta(3)\delta(1-x). \end{aligned} \quad (3.66)$$

The relations in eq. (3.66) can be obtained rearranging, in Mellin space, the terms in such a way to reconstruct the Mellin-transform of well-known terms.

Now, given the LO splitting functions (with expansion parameter $\alpha_s/4\pi$ and such that they can be used to evolve the singlet combination $\{q^+, g\}$):

$$\begin{aligned} P_{qq}^{(0)}(x) &= 2C_F \left[2 \left(\frac{1}{1-x} \right)_+ - (1+x) + \frac{3}{2}\delta(1-x) \right], \\ P_{gg}^{(0)}(x) &= 4n_f T_R [x^2 + (1-x)^2], \\ P_{gq}^{(0)}(x) &= 2C_F \left[\frac{1 + (1-x)^2}{x} \right], \\ P_{qg}^{(0)}(x) &= 4C_A \left[\left(\frac{1}{1-x} \right)_+ - 2 + x - x^2 + \frac{1}{x} \right] + \frac{11C_A - 4n_f T_R}{3} \delta(1-x), \end{aligned} \quad (3.67)$$

we can compute the additional terms involving only combinations of splitting functions. In particular, we need to compute:

$$P_{qq}^{(0)}(x) \otimes P_{qq}^{(0)}(x), \quad (3.68)$$

involved in the $\mathcal{O}(\alpha_s^2)$ non-singlet coefficient functions, and:

$$\begin{aligned} P_{qg}^{(0)}(x) \otimes P_{qg}^{(0)}(x), \\ P_{qi}^{(0)}(x) \otimes P_{ig}^{(0)}(x) = P_{qq}^{(0)}(x) \otimes P_{qg}^{(0)}(x) + P_{qg}^{(0)}(x) \otimes P_{gg}^{(0)}(x). \end{aligned} \quad (3.69)$$

present in the pure-singlet and in the gluon coefficient functions, respectively.

The convolution in eq. (3.68) can be easily computed by hand using eqs. (3.65) and (3.66) and the result is:

$$\begin{aligned}
P_{qq}^{(0)}(x) \otimes P_{qq}^{(0)}(x) &= 4C_F^2 \left[8 \left(\frac{\ln(1-x)}{1-x} \right)_+ + 6 \left(\frac{1}{1-x} \right)_+ - 4 \frac{\ln(x)}{1-x} - 4(1+x) \ln(1-x) \right. \\
&\quad \left. + 3(1+x) \ln(x) - (x+5) + \left(\frac{9}{4} - 4\zeta(2) \right) \delta(1-x) \right].
\end{aligned} \tag{3.70}$$

As for eq. (3.69), where no convolutions of the kinds given in eqs. (3.65) and (3.66) are present, we can safely use Mathematica, obtaining:

$$\begin{aligned}
P_{qg}^{(0)}(x) \otimes P_{qg}^{(0)}(x) &= C_F n_f T_R \left[\frac{8}{3} \left(-4x^2 - 3x + \frac{4}{x} + 3 \right) + 16(x+1) \ln(x) \right], \\
P_{qi}^{(0)}(x) \otimes P_{ig}^{(0)}(x) &= n_f T_R C_A \left[16(2x^2 - 2x + 1) \ln(1-x) + 16(4x+1) \ln(x) + \frac{4}{3} \left(-40x^2 + 26x + 17 + \frac{8}{x} \right) \right] \\
&\quad + n_f T_R C_F \left[16(2x^2 - 2x + 1) \ln(1-x) - 8(4x^2 - 2x + 1) \ln(x) + 4(4x-1) \right] \\
&\quad + n_f^2 T_R^2 \left[-\frac{16}{3}(2x^2 - 2x + 1) \right]
\end{aligned} \tag{3.71}$$

Now we need to consider the additional terms involving combinations of splitting functions and coefficient functions. Let us start considering F_L and it is the easiest case. Here we have:

$$\begin{aligned}
C_{L,\pm}^{(1)}(x) &= 4C_F x, \\
C_{L,q}^{(1)}(x) &= \frac{1}{n_f} C_{L,\pm}^{(1)}(x), \\
C_{L,g}^{(1)}(x) &= 4T_R x(1-x),
\end{aligned} \tag{3.72}$$

and for the non-singlet case we need to compute:

$$C_{L,\pm}^{(1)}(x) \otimes P_{qq}^{(0)}(x) = 4C_F^2 [(x+2) + 4x \ln(1-x) - 2x \ln(x)]. \tag{3.73}$$

For the pure-singlet and the gluon coefficient functions, instead, we need to compute:

$$\begin{aligned}
C_{L,g}^{(1)}(x) \otimes P_{qq}^{(0)}(x) &= C_F T_R \left[\frac{32}{3} \left(2x^2 - 3 + \frac{1}{x} \right) - 32x \ln(x) \right], \\
C_{L,i}^{(1)}(x) \otimes P_{ig}^{(0)}(x) &= C_A T_R \left[64x(1-x) \ln(1-x) - 128x \ln(x) + \frac{16}{3} \left(23x^2 - 19x - 6 + \frac{2}{x} \right) \right] \\
&\quad + C_F T_R \left[\frac{16}{3} x \ln(x) - \frac{8}{3} (2x^2 - x - 1) \right] \\
&\quad + n_f T_R^2 \left[-\frac{64}{3} x(1-x) \right].
\end{aligned} \tag{3.74}$$

Now we consider F_2 , for which we have:

$$\begin{aligned}
C_{2,\pm}^{(1)}(x) &= 2C_F \left[2 \left(\frac{\ln(1-x)}{1-x} \right)_+ - \frac{3}{2} \left(\frac{1}{1-x} \right)_+ - 2 \frac{\ln(x)}{1-x} - (x+1) [\ln(1-x) - \ln(x)] \right. \\
&\quad \left. + 2x + 3 - \left(2\zeta(2) + \frac{9}{2} \right) \delta(1-x) \right],
\end{aligned} \tag{3.75}$$

$$C_{2,q}^{(1)}(x) = \frac{1}{n_f} C_{\pm,2}^{(1)}(x),$$

$$C_{2,g}^{(1)}(x) = 4T_R [(x^2 + (1-x)^2) [\ln(1-x) - \ln(x)] - 8x^2 + 8x - 1].$$

Also in this case we need to compute $C_{2,\pm}^{(1)}(x) \otimes P_{qq}^{(0)}(x)$ and $C_{2,i}^{(1)}(x) \otimes P_{ig}^{(0)}(x)$.

4 Implementation of the Semi-Inclusive e^+e^- Annihilation

The implementation of the Semi-Inclusive e^+e^- Annihilation (SIA) in APFEL is not very complicated. The reason for that is the fact that SIA is structurally identical to DIS. In fact, we can regard SIA as the time-like counterpart of DIS and the differences are only at the level of coefficient functions and splitting functions. Considering that APFEL already implement the time-like evolution [7] (*i.e.* the time-like splitting functions), the only thing to do is implement the respective coefficient functions. Presently the coefficient functions for SIA are known up to $\mathcal{O}(\alpha_s^2)$ (NNLO) in the zero-mass scheme and they have been computed in Ref. [8] and the x -space expressions of interest for the implementation in APFEL reported in Appendix C.

The way in which the SIA expressions are reported is slightly different from the standard way in which we are used to see the DIS expressions. We would like to reduce the SIA expressions to the same form of DIS in such a way to use the DIS module of APFEL also for the SIA cross sections. In particular the SIA cross section is Ref. [8] expressed in terms of the three structure functions: F_T , F_L and F_A . However, comparing the SIA cross section with the DIS cross sections it is easy to realize that defining:

$$\begin{aligned} F_2(x, Q) &= F_T(x, Q) + F_L(x, Q), \\ F_L(x, Q) &= F_L(x, Q), \\ F_A(x, Q) &= xF_3(x, Q), \end{aligned} \tag{4.1}$$

the SIA cross section reduces to the same structure of the DIS cross section.

Assuming that:

$$F_k(x, Q) = \sum_{j=q,g} x \int_x^1 \frac{dy}{y} c_{k,j}(\alpha_s(Q), x) \mathcal{D}_j\left(\frac{x}{y}, Q\right), \quad \text{with } k = 2, L, 3, \tag{4.2}$$

(note that, to uniform the notation, we understood the factor x in front of F_3) where \mathcal{D}_j is the fragmentation function of the flavour j and where the coefficient functions $c_{k,j}$ allow for the perturbative expansion:

$$c_{k,j}(\alpha_s(Q), x) = \sum_{n=0}^N \alpha_s^n(Q) c_{k,j}^{(n)}(x), \tag{4.3}$$

we have that the leading-order coefficient functions are trivially:

$$\begin{aligned} c_{k,g}^{(0)}(x) &= 0, \quad k = 2, L, 3, \\ c_{L,q}^{(0)}(x) &= 0, \\ c_{2,q}^{(0)}(x) &= c_{3,q}^{(0)}(x) = \delta(1-x). \end{aligned} \tag{4.4}$$

Now we consider the NLO coefficient functions. Their explicit expressions are give in eqs. (C.13)-(C.17) of Ref. [8] but, in order to write them in a form suitable for the implementation in APFEL, we need to isolate the regular, soft-divergent and local terms and finally combine them according to eq. (4.1).

$$\begin{aligned}
c_{L,q}^{(1)}(x) &= 2C_F \\
c_{L,g}^{(1)}(x) &= 2C_F \frac{4(1-x)}{x} \\
c_{2,q}^{(1)}(x) = c_{T,q}^{(1)}(x) + c_{L,q}^{(1)}(x) &= 2C_F \left[2 \left(\frac{\ln(1-x)}{1-x} \right)_+ - \frac{3}{2} \left(\frac{1}{1-x} \right)_+ - (1+x) \ln(1-x) \right. \\
&\quad \left. + 2 \frac{1+x^2}{1-x} \ln x + \frac{5}{2} - \frac{3}{2}x + \left(4\zeta_2 - \frac{9}{2} \right) \delta(1-x) \right] \\
c_{2,g}^{(1)}(x) = c_{T,g}^{(1)}(x) + c_{L,g}^{(1)}(x) &= 4C_F \frac{1+(1-x)^2}{x} \ln[x^2(1-x)] \\
c_{3,q}^{(1)}(x) &= 2C_F \left[2 \left(\frac{\ln(1-x)}{1-x} \right)_+ - \frac{3}{2} \left(\frac{1}{1-x} \right)_+ - (1+x) \ln(1-x) \right. \\
&\quad \left. + 2 \frac{1+x^2}{1-x} \ln x + \frac{1}{2} - \frac{1}{2}x + \left(4\zeta_2 - \frac{9}{2} \right) \delta(1-x) \right] \\
c_{3,g}^{(1)}(x) &= 0
\end{aligned} \tag{4.5}$$

It is interesting to notice that, as expected, the soft-singular part of the quark coefficient functions is exactly the same as in DIS and this allows us to reuse part of the DIS coefficient functions.

5 Polarized DIS cross section and structure functions

Let us consider the differential cross sections for unpolarized and polarized Deep-Inelastic Scattering (DIS) (see *e.g.* Eq. (19.16) of Sec. 19 in Ref. [9]):

$$\begin{aligned}
\frac{d^2\sigma^i}{dxdy} &= \frac{2\pi\alpha^2}{xyQ^2} \eta^i [Y_+ F_2^i \mp Y_- x F_3^i - y^2 F_L^i] \\
\frac{d^2\Delta\sigma^i}{dxdy} &= \frac{2\pi\alpha^2}{xyQ^2} \eta^i [-Y_+ g_4^i \mp Y_- 2xg_1^i + y^2 g_L^i] ,
\end{aligned} \tag{5.1}$$

where $i = \text{NC, CC}$, $Y_{\pm} = 1 \pm (1-y)^2$, $\eta^{\text{NC}} = 1$, $\eta^{\text{CC}} = (1 \pm \lambda)^2 \eta_W$ (with $\lambda = \pm 1$ is the helicity of the incoming lepton and $\eta_W = \frac{1}{2} \left(\frac{G_F M_W}{4\pi\alpha} \frac{Q^2}{Q^2 + M_W^2} \right)^2$), and

$$\begin{aligned}
F_L^i &= F_2^i - 2xF_1^i \\
F_L^i &= g_4^i - 2xg_5^i .
\end{aligned} \tag{5.2}$$

Because the same tensor structure occurs in the spin-dependent and spin-independent parts of the DIS hadronic tensor (in the limit $M^2/Q^2 \rightarrow 0$), the polarized cross section can be obtained from the unpolarized cross section with the following replacement

$$F_2^i \rightarrow -2g_4^i \quad F_3^i \rightarrow +4g_1^i \quad F_L^i \rightarrow -2g_L^i . \tag{5.3}$$

Note that the extra factor two is due to the fact that the total cross section is an average over initial-state polarizations.

The *polarized* structure functions g_4 , g_1 and g_L are expressed as a convolution of coefficient functions, $\Delta c_{k,j}$, and polarized PDFs, Δf_j , (summed over all flavors j)

$$g_k(x, Q) = \sum_{j=q,g} x \int_x^1 \frac{dy}{y} \Delta c_{k,j}(\alpha_s(Q), x) \Delta f_j\left(\frac{x}{y}, Q\right) , \quad \text{with } k = 4, 1, L . \tag{5.4}$$

The coefficient functions $\Delta c_{k,j}$ allow for the usual perturbative expansion

$$\Delta c_{k,j}(\alpha_s(Q), x) = \sum_{n=0}^N \left(\frac{\alpha_s(Q)}{4\pi} \right)^n \Delta c_{k,j}^{(n)}(x), \quad (5.5)$$

where the coefficients $\Delta c_{k,j}^{(n)}(x)$ are known up to NLO, *i.e.* $n = 1$ (see *e.g.* [10] and references therein). At LO they are

$$\begin{aligned} \Delta c_{4,q}^{(0)}(x) &= \Delta c_{1,q}^{(0)}(x) &= \delta(1-x) \\ \Delta c_{L,q}^{(0)}(x) &= 0, \\ \Delta c_{k,g}^{(0)}(x) &= 0 \quad \text{with } k = 4, 1, L. \end{aligned} \quad (5.6)$$

At NLO they read

$$\begin{aligned} \Delta c_{4,q}^{(1)}(x) &= 2C_F \left\{ 2 \left[\frac{\ln(1-x)}{1-x} \right]_+ - \frac{3}{2} \left[\frac{1}{1-x} \right]_+ - (1+x) \ln(1-x) \right. \\ &\quad \left. - \frac{1+x^2}{1-x} \ln x + 3 + 2x - \left(\frac{9}{2} + 2\zeta_2 \right) \delta(1-x) \right\}, \\ \Delta c_{4,g}^{(1)}(x) &= 0, \\ \Delta c_{1,q}^{(1)}(x) &= 2C_F \left\{ 2 \left[\frac{\ln(1-x)}{1-x} \right]_+ - \frac{3}{2} \left[\frac{1}{1-x} \right]_+ - (1+x) \ln(1-x) \right. \\ &\quad \left. - \frac{1+x^2}{1-x} \ln x + 2 + x - \left(\frac{9}{2} + 2\zeta_2 \right) \delta(1-x) \right\}, \\ \Delta c_{1,g}^{(1)}(x) &= 4T_R \left\{ (2x-1) \ln \frac{1-x}{x} - 4x + 3 \right\}, \\ \Delta c_{L,q}^{(1)}(x) &= 2C_F 2x, \\ \Delta c_{L,g}^{(1)}(x) &= 0. \end{aligned} \quad (5.7)$$

In the NC case the couplings can be written as:

$$\begin{aligned} B_q(Q^2) &= -e_q A_q (V_e \pm \lambda A_e) P_Z + V_q A_q (V_e^2 + A_e^2 \pm 2\lambda V_e A_e) P_Z^2, \\ D_q(Q^2) &= \pm \frac{1}{2} \lambda e_q^2 - e_q V_q (A_e \pm \lambda V_e) P_Z + \frac{1}{2} (V_q^2 + A_q^2) [2V_e A_e \pm \lambda (V_e^2 + A_e^2)] P_Z^2. \end{aligned} \quad (5.8)$$

where λ corresponds to the polarization of the incoming lepton. It should be stressed that B_q multiplies g_4 and g_L while D_q multiplies g_1 .

6 The χ Prescription in FONLL

As is well known, the original formulation of the FONLL matched scheme gives rise to discontinuities in correspondence of the heavy quark thresholds arising from uncontrolled subleading terms. Such subleading terms can however be numerically important especially around the charm threshold where the numerical value of the strong coupling α_s is large. In order to remedy this unwanted feature different prescriptions have been introduced and traditionally the FONLL schem DIS has been implemented using the so-called damping factor which directly suppresses the unwanted subleading terms by means of a function that goes smoothly to zero at the threshold and below and tends to one for energies much larger than the threshold itself.

As an alternative to the damping factor, one can damp the subleading terms close to the threshold by mimicing in the subtraction terms the phase-space suppression given by the presence of one or more heavy

quarks in the final state. This is easily done just by introducing the so-called slow-rescaling variable χ , that in the NC case is:

$$\chi = x \left(1 + \frac{4m_H^2}{Q^2} \right) = \frac{x}{\eta}, \quad (6.1)$$

m_H being the mass of the heavy quark, in the convolution between coefficient functions and PDFs in the zero-mass and in the massless-limit bits of the FONLL structure function. In other words, the usual zero-mass Mellin convolution becomes:

$$x \int_x^1 \frac{dy}{y} C\left(\frac{x}{y}\right) f(y) \rightarrow x \int_\chi^1 \frac{dy}{y} C\left(\frac{\chi}{y}\right) f(y) = x \int_\chi^1 \frac{dy}{y} C(y) f\left(\frac{\chi}{y}\right). \quad (6.2)$$

The question is how to treat the new integral on a discrete x -space grid. What we have done so far for the massive integrals like that in the r.h.s. of the equation above is re-express it in terms of the physical Bjorken x as:

$$x \int_\chi^1 \frac{dy}{y} C(y) f\left(\frac{\chi}{y}\right) \quad (6.3)$$

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