

# 1 Structure of the observables

Let us start from Eq. (2.6) of Ref. [1], that is the fully differential cross section for lepton-pair production in the region in which the TMD factorisation applies, *i.e.*  $q_T \ll Q$ . After some minor manipulations, it reads:

$$\frac{d\sigma}{dQ dy dq_T} = \frac{16\pi\alpha^2 q_T}{9Q^3} H(Q, \mu) \sum_q C_q(Q) \int \frac{d^2\mathbf{b}}{4\pi} e^{i\mathbf{b}\cdot\mathbf{q}_T} \bar{F}_q(x_1, \mathbf{b}; \mu, \zeta) \bar{F}_{\bar{q}}(x_2, \mathbf{b}; \mu, \zeta), \quad (1)$$

where  $Q$ ,  $y$ , and  $q_T$  are the invariant mass, the rapidity, and the transverse momentum of the lepton pair, respectively, while  $\alpha$  is the electromagnetic coupling,  $H$  is the appropriate QCD hard factor that can be perturbatively computed, and  $C_q$  are the effective electroweak charges. In addition, the variables  $x_1$  and  $x_2$  are functions of  $Q$  and  $y$  and are given by:

$$x_{1,2} = \frac{Q}{\sqrt{s}} e^{\pm y}, \quad (2)$$

being  $\sqrt{s}$  the centre-of-mass energy of the collision. In Eq. (1) we are using the short-hand notation:

$$\bar{F}_q(x, \mathbf{b}; \mu, \zeta) \equiv x F_q(x, \mathbf{b}; \mu, \zeta), \quad (3)$$

that is convenient for the implementation. The scales  $\mu$  and  $\zeta$  are introduced as a consequence of the removal of UV and rapidity divergences in the definition of the TMDs. Despite these scales are arbitrary scales, they are typically chosen  $\mu = \sqrt{\zeta} = Q$ . Therefore, for all practical purposes their presence is fictitious.

The computation-intensive part of Eq.(1) has the form of the integral:

$$I_{ij}(x_1, x_2, q_T; \mu, \zeta) = \int \frac{d^2\mathbf{b}}{4\pi} e^{i\mathbf{b}\cdot\mathbf{q}_T} \bar{F}_i(x_1, \mathbf{b}; \mu, \zeta) \bar{F}_j(x_2, \mathbf{b}; \mu, \zeta). \quad (4)$$

where  $\bar{F}_{i(j)}$  are combinations of evolved TMD PDFs. At this stage, for convenience,  $i$  and  $j$  do not coincide with  $q$  and  $\bar{q}$  but they are linked through a simple linear transformation. The integral over the bidimensional impact parameter  $\mathbf{b}$  has to be taken. However,  $\bar{F}_{i(j)}$  only depend on the absolute value of  $\mathbf{b}$ , therefore Eq. (4) can be written as:

$$I_{ij}(x_1, x_2, q_T; \mu, \zeta) = \frac{1}{2} \int_0^\infty db b J_0(b q_T) \bar{F}_i(x_1, b; \mu, \zeta) \bar{F}_j(x_2, b; \mu, \zeta). \quad (5)$$

where  $J_0$  is the zero-th order Bessel function of the first kind whose integral representation is:

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{ix \cos(\theta)}. \quad (6)$$

The evolved quark TMD PDF  $\bar{F}_i$  at the final scales  $\mu$  and  $\zeta$  is obtained by multiplying the same distribution at the initial scales  $\mu_0$  and  $\zeta_0$  by a single evolution factor  $R_q$ <sup>(1)</sup>. that is:

$$\bar{F}_i(x, b; \mu, \zeta) = R_q(\mu_0, \zeta_0 \rightarrow \mu, \zeta; b) \bar{F}_i(x, b; \mu_0, \zeta_0). \quad (7)$$

The initial scale TMD PDFs at small values  $b$  can be written as:

$$\bar{F}_i(x, b; \mu_0, \zeta_0) = \sum_{j=g, q(\bar{q})} x \int_x^1 \frac{dy}{y} C_{ij}(y; \mu_0, \zeta_0) f_j\left(\frac{x}{y}, \mu_0\right), \quad (8)$$

where  $f_j$  are the collinear PDFs (including the gluon) and  $C_{ij}$  are the so-called matching functions that are perturbatively computable and are currently known to NNLO, *i.e.*  $\mathcal{O}(\alpha_s^2)$ . If we define:

$$\bar{f}_i(x, \mu_0) = x f_i(x, \mu_0), \quad (9)$$

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<sup>1</sup>Note that in Eq. (1) the gluon TMD PDF  $\bar{F}_g$  is not involved. If also the gluon TMD PDF was involved, it would evolve by means of a different evolution factor  $R_g$ .

Eq. (8) can be written as:

$$\bar{F}_i(x, b; \mu_0, \zeta_0) = \sum_{j=g, q(\bar{q})} \int_x^1 dy C_{ij}(y; \mu_0, \zeta_0) \bar{f}_i\left(\frac{x}{y}, \mu_0\right). \quad (10)$$

Putting Eqs. (7) and (10), one finds:

$$\bar{F}_i(x, b; \mu, \zeta) = R_q(\mu_0, \zeta_0 \rightarrow \mu, \zeta; b) \sum_{j=g, q(\bar{q})} \int_x^1 dy C_{ij}(y; \mu_0, \zeta_0) \bar{f}_i\left(\frac{x}{y}, \mu_0\right). \quad (11)$$

Matching and evolution are affected by non-perturbative effects that become relevant at large  $b$ . In order to account for such effects, one usually introduces a phenomenological function  $f_{\text{NP}}$ . In the traditional approach (CSS [2]), the  $b$ -space TMDs get a multiplicative correction that does not depend on the flavour. In addition, the perturbative content of the TMDs is smoothly damped away at large  $b$  by introducing the so-called  $b_*$ -prescription:

$$\bar{F}_i(x, b; \mu, \zeta) \rightarrow \bar{F}_i(x, b_*(b); \mu, \zeta) f_{\text{NP}}(x, b, \zeta), \quad (12)$$

where  $b_* \equiv b_*(b)$  is a monotonic function of the impact parameter  $b$  such that:

$$\lim_{b \rightarrow 0} b_*(b) = b_{\min} \quad \text{and} \quad \lim_{b \rightarrow \infty} b_*(b) = b_{\max}, \quad (13)$$

being  $b_{\min}$  and  $b_{\max}$  constant values both in the perturbative region. Including the non-perturbative function, Eq. (5) becomes:

$$\begin{aligned} I_{ij}(x_1, x_2, q_T; \mu, \zeta) &= \int_0^\infty db J_0(b q_T) \left[ \frac{b}{2} \bar{F}_i(x_1, b_*(b); \mu, \zeta) \bar{F}_j(x_2, b_*(b); \mu, \zeta) f_{\text{NP}}(x_1, b, \zeta) f_{\text{NP}}(x_2, b, \zeta) \right] \\ &= \frac{1}{q_T} \int_0^\infty d\bar{b} J_0(\bar{b}) \left[ \frac{\bar{b}}{2 q_T} \bar{F}_i(x_1, b_*\left(\frac{\bar{b}}{q_T}\right); \mu, \zeta) \bar{F}_j(x_2, b_*\left(\frac{\bar{b}}{q_T}\right); \mu, \zeta) f_{\text{NP}}\left(x_1, \frac{\bar{b}}{q_T}, \zeta\right) f_{\text{NP}}\left(x_2, \frac{\bar{b}}{q_T}, \zeta\right) \right]. \end{aligned} \quad (14)$$

Eq. (14) is a Hankel tranform and can be efficiently computed using the so-called Ogata quadrature [3]. Effectively, the computation of the integral in Eq. (4) is achieved through a weighted sum:

$$\begin{aligned} I_{ij}(x_1, x_2, q_T; \mu, \zeta) &\simeq \frac{1}{q_T} \sum_{n=1}^N \frac{w_n^{(0)} z_n^{(0)}}{2 q_T} \bar{F}_i\left(x_1, b_*\left(\frac{z_n^{(0)}}{q_T}\right); \mu, \zeta\right) \bar{F}_j\left(x_2, b_*\left(\frac{z_n^{(0)}}{q_T}\right); \mu, \zeta\right) \\ &\times f_{\text{NP}}\left(x_1, \frac{z_n^{(0)}}{q_T}, \zeta\right) f_{\text{NP}}\left(x_2, \frac{z_n^{(0)}}{q_T}, \zeta\right), \end{aligned} \quad (15)$$

where the unscaled coordinates  $z_n^{(0)}$  and the weights  $w_n^{(0)}$  can be precomputed in terms of the zero's of the Bessel function  $J_0$  and one single parameter (see Ref. [3] for more details, specifically Eqs. (5.1) and (5.2) or Appendix A for the relevant formula to compute the unscaled coordinates and the weights)<sup>2</sup>. Based on the (empirically verified) assumption that the absolute value of each term in the sum in the r.h.s. of Eq. (15) is smaller than that of the preceding one, the truncation number  $N$  is chosen dynamically in such a way that the  $(N+1)$ -th term is smaller in absolute value than a user-defined cutoff relatively to the sum of the preceding  $N$  terms.

Eq. (15) factors out the non-perturbative part of the calculation represented by  $f_{\text{NP}}$  from the perturbative content. This is done on purpose to devise a method in which the perturbative content

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<sup>2</sup>The superscript 0 in  $z_n^{(0)}$  and  $w_n^{(0)}$  indicates that here we are performing a Hankel tranform that involves the Bessel function of degree zero  $J_0$ . This is useful in view of the next section in which the integration over  $q_T$  will give rise to a similar Hankel transform with  $J_0$  replaced by  $J_1$ . Also in that case the Ogata quadrature algorithm can be applied but coordinates and weights will be different.

is precomputed and numerically convoluted with the non-perturbative functions *a posteriori*. This is convenient in view of a fit of the function  $f_{\text{NP}}$ .

As customary in QCD, the most convenient basis for the matching in Eq. (8) is the so-called “evolution” basis (*i.e.*  $\Sigma$ ,  $V$ ,  $T_3$ ,  $V_3$ , etc.). In fact, in this basis the operator matrix  $C_{ij}$  is almost diagonal with the only exception of crossing terms that couple the gluon and the singlet  $\Sigma$  distributions. As a consequence, this is the most convenient basis for the computation of  $I_{ij}$ . On the other hand, TMDs in Eq. (1) appear in the so-called “physical” basis (*i.e.*  $d$ ,  $\bar{d}$ ,  $u$ ,  $\bar{u}$ , etc.). Therefore, we need to rotate  $F_{i(j)}$  from the evolution basis, over which the indices  $i$  and  $j$  run, to the physical basis. This is done by means of an appropriate constant matrix  $T$ , so that:

$$\bar{F}_q(x_1, b; \mu, \zeta) = \sum_i T_{qi} F_i(x_1, b; \mu, \zeta), \quad (16)$$

and similarly for  $\bar{F}_{\bar{q}}$ . Putting all pieces together, one can conveniently write the cross section in Eq. (1) as:

$$\frac{d\sigma}{dQ dy dq_T} \simeq \sum_{n=1}^N w_n^{(0)} \frac{z_n^{(0)}}{q_T} S\left(x_1, x_2, \frac{z_n^{(0)}}{q_T}; \mu, \zeta\right) f_{\text{NP}}\left(x_1, \frac{z_n^{(0)}}{q_T}, \zeta\right) f_{\text{NP}}\left(x_2, \frac{z_n^{(0)}}{q_T}, \zeta\right), \quad (17)$$

with:

$$S(x_1, x_2, b; \mu, \zeta) = \frac{8\pi\alpha^2}{9Q^3} H(Q, \mu) \sum_q C_q(Q) [\bar{F}_q(x_1, b_*(b); \mu, \zeta)] [\bar{F}_{\bar{q}}(x_2, b_*(b); \mu, \zeta)]. \quad (18)$$

Eq. (17) allows one to precompute the weights  $S$  in such a way that the differential cross section in Eq. (1) can be computed as a simple weighted sum of the non-perturbative contribution. A misleading aspect of Eq. (18) is the fact that  $S$  has five arguments. In actual facts,  $S$  only depends on three independent variables. The reason is that  $\mu$  and  $\zeta$  are usually taken to be proportional to  $Q$  by a constant factor. In addition  $x_1$  and  $x_2$  depend on  $Q$  and  $y$  through Eq. (2). Therefore, the full dependence on the kinematics of the final state of Eq. (1) can be specified by  $Q$ ,  $y$  and  $q_T$ .

## 2 Integrating over the final-state kinematic variables

Despite Eq. (17) provides a powerful tool for a fast computation of cross sections, it is often not sufficient to allow for a direct comparison to experimental data. The reason is that experimental measurements of differential distributions are usually delivered as integrated over finite regions of the final-state kinematic phase space. In other words, experiments measure quantities like:

$$\tilde{\sigma} = \int_{Q_{\min}}^{Q_{\max}} dQ \int_{y_{\min}}^{y_{\max}} dy \int_{q_{T,\min}}^{q_{T,\max}} dq_T \left[ \frac{d\sigma}{dQ dy dq_T} \right]. \quad (19)$$

As a consequence, in order to guarantee performance, we need to include the integrations above in the precomputed factors.

### 2.1 Integrating over $q_T$

The integration over bins in  $q_T$  can be carried out analytically exploiting the following property of Bessel’s function:

$$\frac{d}{dx} [x^m J_m(x)] = x^m J_{m-1}(x), \quad (20)$$

that leads to:

$$\int dx x J_0(x) = x J_1(x) \quad \Rightarrow \quad \int_{x_1}^{x_2} dx x J_0(x) = x_2 J_1(x_2) - x_1 J_1(x_1). \quad (21)$$

To see it, we observe that the differential cross section in Eq. (1) has the following structure:

$$\frac{d\sigma}{dQdydq_T} \propto \int_0^\infty db \, q_T J_0(bq_T) \dots \quad (22)$$

where the ellipses indicate terms that do not depend on  $q_T$ . Therefore, using Eq. (21) we find:

$$\begin{aligned} \int_{q_{T,\min}}^{q_{T,\max}} dq_T \left[ \frac{d\sigma}{dQdydq_T} \right] &\propto \int_0^\infty db \int_{q_{T,\min}}^{q_{T,\max}} dq_T \, q_T J_0(bq_T) \dots = \\ &\int_0^\infty \frac{db}{b^2} \int_{bq_{T,\min}}^{bq_{T,\max}} dx \, x J_0(x) \dots = \int_0^\infty \frac{db}{b} [q_{T,\max} J_1(bq_{T,\max}) - q_{T,\min} J_1(bq_{T,\min})] \dots \end{aligned} \quad (23)$$

Therefore, defining:

$$K(q_T) \equiv \int dq_T \left[ \frac{d\sigma}{dQdydq_T} \right] \quad (24)$$

as the indefinite integral over  $q_T$  of the cross section in Eq. (1), we have that:

$$\int_{q_{T,\min}}^{q_{T,\max}} dq_T \left[ \frac{d\sigma}{dQdydq_T} \right] = K(Q, y, q_{T,\max}) - K(Q, y, q_{T,\min}), \quad (25)$$

with:

$$\begin{aligned} K(Q, y, q_T) &= \frac{8\pi\alpha^2 q_T}{9Q^3} H(Q, \mu) \\ &\times \int_0^\infty db \, J_1(bq_T) \sum_q C_q(Q) \bar{F}_q(x_1, b; \mu, \zeta) \bar{F}_{\bar{q}}(x_2, b; \mu, \zeta) f_{\text{NP}}(x_1, b, \zeta) f_{\text{NP}}(x_2, b, \zeta), \end{aligned} \quad (26)$$

that can be computed using the Ogata quadrature as:

$$K(Q, y, q_T) \simeq \sum_{n=1}^N w_n^{(1)} S \left( x_1, x_2, \frac{z_n^{(1)}}{q_T}; \mu, \zeta \right) f_{\text{NP}} \left( x_1, \frac{z_n^{(1)}}{q_T}, \zeta \right) f_{\text{NP}} \left( x_2, \frac{z_n^{(1)}}{q_T}, \zeta \right), \quad (27)$$

with  $S$  defined in Eq. (18). The unscaled coordinates  $z_n^{(1)}$  and the weights  $w_n^{(1)}$  can again be precomputed and stored in terms of the zero's of the Bessel function  $J_1$ . Eq. (25) reduces the integration in  $q_T$  to a calculation completely analogous to the unintegrated cross section. This is particularly convenient because it avoids the computation a numerical integration.

### 2.1.1 Kinematic cuts

In the presence of kinematic cuts, such as those on the final-state leptons in Drell-Yan, the analytic integration over  $q_T$  discussed above cannot be performed. The reason is that the implementation of these cuts effectively introduces a  $q_T$ -dependent function  $\mathcal{P}$ <sup>(3)</sup> in the integral:

$$\frac{d\sigma}{dQdydq_T} \propto \int_0^\infty db \, q_T J_0(bq_T) \mathcal{P}(q_T) \dots, \quad (28)$$

that prevents the direct use of Eq. (21). Since  $\mathcal{P}$  is a slowly-varying function of  $q_T$  over the typical bin size, we can approximate the integral over the bins in  $q_T$  as:

$$\begin{aligned} \int_{q_{T,\min}}^{q_{T,\max}} dq_T \, q_T J_0(bq_T) \mathcal{P}(q_T) &\simeq \mathcal{P} \left( \frac{q_{T,\max} + q_{T,\min}}{2} \right) \int_{q_{T,\min}}^{q_{T,\max}} dq_T \, q_T J_0(bq_T) \\ &= \mathcal{P} \left( \frac{q_{T,\max} + q_{T,\min}}{2} \right) \frac{1}{b} [q_{T,\max} J_1(bq_{T,\max}) - q_{T,\min} J_1(bq_{T,\min})]. \end{aligned} \quad (29)$$

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<sup>3</sup>In fact,  $\mathcal{P}$  also depends on the invariant mass  $Q$  and the rapidity  $y$  of the lepton pair that also need to be integrated over.

Unfortunately, this structure is inconvenient because it mixes different bin bounds and prevents a recursive computation. However, we can try to go further and, assuming that the bin width is small enough, we can expand  $\mathcal{P}$  in the following ways:

$$\begin{aligned}\mathcal{P}\left(\frac{q_{T,\max} + q_{T,\min}}{2}\right) &= \mathcal{P}(q_{T,\min} + \Delta q_T) = \mathcal{P}(q_{T,\min}) + \mathcal{P}'(q_{T,\min}) \Delta q_T + \mathcal{O}(\Delta q_T^2), \\ \mathcal{P}\left(\frac{q_{T,\max} + q_{T,\min}}{2}\right) &= \mathcal{P}(q_{T,\max} - \Delta q_T) = \mathcal{P}(q_{T,\max}) - \mathcal{P}'(q_{T,\max}) \Delta q_T + \mathcal{O}(\Delta q_T^2),\end{aligned}\tag{30}$$

with:

$$\Delta q_T = \frac{q_{T,\max} - q_{T,\min}}{2}.\tag{31}$$

Therefore:

$$\begin{aligned}b \int_{q_{T,\min}}^{q_{T,\max}} dq_T q_T J_0(bq_T) \mathcal{P}(q_T) &\simeq q_{T,\max} J_1(bq_{T,\max}) [\mathcal{P}(q_{T,\max}) - \mathcal{P}'(q_{T,\max}) \Delta q_T] \\ &- q_{T,\min} J_1(bq_{T,\min}) [\mathcal{P}(q_{T,\min}) + \mathcal{P}'(q_{T,\min}) \Delta q_T].\end{aligned}\tag{32}$$

The advantage of this formula as compared to Eq. (29) is that each single term depends on one single bin-bound in  $q_T$  rather than on a combination of two consecutive bounds. Therefore, in the presence of kinematic cuts, the actual form of the primitive function  $K$  defined in Eq. (25) and given explicitly in Eq. (26) is:

$$\begin{aligned}K(Q, y, q_T) &= \frac{8\pi\alpha^2 q_T}{9Q^3} H(Q, \mu) [\mathcal{P}(Q, y, q_T) \pm \mathcal{P}'(Q, y, q_T) \Delta q_T] \\ &\times \int_0^\infty db J_1(bq_T) \sum_q C_q(Q) \bar{F}_q(x_1, b; \mu, \zeta) \bar{F}_{\bar{q}}(x_2, b; \mu, \zeta) f_{\text{NP}}(x_1, b, \zeta) f_{\text{NP}}(x_2, b, \zeta),\end{aligned}\tag{33}$$

where I have explicitly reinstated the dependence of the function  $\mathcal{P}$  and its derivative with respect to  $q_T$ ,  $\mathcal{P}'$ , on  $Q$  and  $y$ . In the square bracket in Eq. (33), the minus sign applies when  $q_T$  is the upper bound of the bin and the plus sign when it is the lower bound (see Eq. (32)). As discussed below, when integrating over bins in  $Q$  and  $y$ , one should also integrate the functions  $\mathcal{P}$  and  $\mathcal{P}'$ . However, we will argue that, in the interpolation procedure discussed below, these functions can be extracted from the integrals in  $Q$  and  $y$  in a proper manner in such a way to avoid computing the expensive function  $\mathcal{P}$  many times and, moreover, simplify enormously the structure of the resulting interpolation tables.

## 2.2 On the position of the peak of the $q_T$ distribution

It is interesting at this point to take a short detour to discuss the position of the peak on the distribution in  $q_T$  of the cross section in Eq. (1). The peak can be located by setting the derivative in  $q_T$  of the cross section equal to zero. To do so, we use another property of Bessel's functions:

$$\frac{dJ_0(x)}{dx} = -J_1(x).\tag{34}$$

Using this relation, it is easy to see that:

$$\begin{aligned}0 &= \frac{d}{dq_T} \left[ \frac{d\sigma}{dQ dy dq_T} \right] = \\ &\frac{8\pi\alpha^2}{9Q^3} H(Q, \mu) \int_0^\infty db b [J_0(bq_T) - bq_T J_1(bq_T)] \sum_q C_q(Q) \bar{F}_q(x_1, b_*(b); \mu, \zeta) \bar{F}_{\bar{q}}(x_2, b_*(b); \mu, \zeta) \\ &\times f_{\text{NP}}(x_1, b, \zeta) f_{\text{NP}}(x_2, b, \zeta),\end{aligned}\tag{35}$$

that is equivalent to require that:

$$\int_0^\infty db b [J_0(bq_T) - bq_T J_1(bq_T)] \sum_q C_q(Q) \bar{F}_q(x_1, b_*(b); \mu, \zeta) \bar{F}_{\bar{q}}(x_2, b_*(b); \mu, \zeta) f_{\text{NP}}(x_1, b, \zeta) f_{\text{NP}}(x_2, b, \zeta) = 0. \quad (36)$$

The integral above can be solved numerically using the technique discussed above and the value of  $q_T$  that satisfies this equation represents the position of the peak of the  $q_T$  distribution.

### 2.3 Integrating over $Q$ and $y$

As a final step, we need to perform the integrals over  $Q$  and  $y$  defined in Eq. (19). To compute these integrals we can only rely on numerical methods. Having reduced the integration in  $q_T$  to the difference of the two terms in the r.h.s. of Eq. (25)<sup>(4)</sup>, we can concentrate on integrating the function  $K$  over  $Q$  and  $y$  for a fixed value of  $q_T$ :

$$\tilde{K}(q_T) = \int_{Q_{\min}}^{Q_{\max}} dQ \int_{y_{\min}}^{y_{\max}} dy K(Q, y, q_T), \quad (37)$$

such that:

$$\tilde{\sigma} = \tilde{K}(q_{T,\max}) - \tilde{K}(q_{T,\min}). \quad (38)$$

To this purpose, it is convenient to make explicit the dependence of  $x_1$  and  $x_2$  on  $Q$  and  $y$  using Eq. (2). In addition, for the sake of simplicity we will identify the scales  $\mu$  and  $\sqrt{\zeta}$  with  $Q$  (possible scale variations can be easily reinstated at a later stage) and thus drop one of the arguments from the TMD distributions  $\bar{F}$  and from the hard factor  $H$ . This yields:

$$\begin{aligned} \tilde{K}(q_T) &= \frac{8\pi q_T}{9} \int_0^\infty db J_1(bq_T) \int_{Q_{\min}}^{Q_{\max}} dQ \int_{e^{y_{\min}}}^{e^{y_{\max}}} \frac{d\xi}{\xi} \\ &\times \frac{1}{Q^3} \alpha^2(Q) H(Q) \sum_q C_q(Q) \bar{F}_q\left(\frac{Q}{\sqrt{s}} \xi, b_*(b); Q\right) \bar{F}_{\bar{q}}\left(\frac{Q}{\sqrt{s}} \frac{1}{\xi}, b_*(b); Q\right) \\ &\times f_{\text{NP}}\left(\frac{Q}{\sqrt{s}} \xi, b; Q\right) f_{\text{NP}}\left(\frac{Q}{\sqrt{s}} \frac{1}{\xi}, b; Q\right), \end{aligned} \quad (39)$$

where we have performed the change of variable  $e^y = \xi$ . Now we define one grid in  $\xi$ ,  $\{\xi_\alpha\}$  with  $\alpha = 0, \dots, N_\xi$ , and one grid in  $Q$ ,  $\{Q_\tau\}$  with  $\tau = 0, \dots, N_Q$ , each of which with a set of interpolating functions  $\mathcal{I}$  associated. In addition, the grids are such that:  $\xi_0 = e^{y_{\min}}$  and  $\xi_{N_\xi} = e^{y_{\max}}$ , and  $Q_0 = Q_{\min}$  and  $Q_{N_Q} = Q_{\max}$ . More details on the interpolation procedure are presented in Appendix B. This allows us to interpolate the pair of functions  $f_{\text{NP}}$  in Eq. (39) for generic values of  $\xi$  and  $Q$  as:

$$f_{\text{NP}}\left(\frac{Q}{\sqrt{s}} \xi, b; Q\right) f_{\text{NP}}\left(\frac{Q}{\sqrt{s}} \frac{1}{\xi}, b; Q\right) \simeq \sum_{\alpha=0}^{N_\xi} \sum_{\tau=0}^{N_Q} \mathcal{I}_\alpha(\xi) \mathcal{I}_\tau(Q) f_{\text{NP}}\left(\frac{Q_\tau}{\sqrt{s}} \xi_\alpha, b; Q_\tau\right) f_{\text{NP}}\left(\frac{Q_\tau}{\sqrt{s}} \frac{1}{\xi_\alpha}, b; Q_\tau\right). \quad (40)$$

Plugging the equation above into Eq. (39) we obtain:

$$\begin{aligned} \tilde{K}(q_T) &\simeq \frac{8\pi q_T}{9} \int_0^\infty db J_1(bq_T) \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_\xi} \left[ \int_{Q_{\min}}^{Q_{\max}} dQ \mathcal{I}_\tau(Q) \frac{1}{Q^3} \alpha^2(Q) H(Q) \right. \\ &\times \left. \int_{e^{y_{\min}}}^{e^{y_{\max}}} d\xi \mathcal{I}_\alpha(\xi) \frac{1}{\xi} \sum_q C_q(Q) \bar{F}_q\left(\frac{Q}{\sqrt{s}} \xi, b_*(b); Q\right) \bar{F}_{\bar{q}}\left(\frac{Q}{\sqrt{s}} \frac{1}{\xi}, b_*(b); Q\right) \right] \\ &\times f_{\text{NP}}\left(\frac{Q_\tau}{\sqrt{s}} \xi_\alpha, b; Q_\tau\right) f_{\text{NP}}\left(\frac{Q_\tau}{\sqrt{s}} \frac{1}{\xi_\alpha}, b; Q_\tau\right). \end{aligned} \quad (41)$$

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<sup>4</sup>For the moment we ignore the complication introduced by the presence of cuts on the final state discussed in Sect. 2.1.1. We will come back on this issue at the end of the section.

Finally, the integration over  $b$  can be performed using the Ogata quadrature as discussed above, so that:

$$\begin{aligned}\tilde{K}(q_T) &\simeq \sum_{n=1}^N \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_\xi} \left[ \frac{8\pi}{9} w_n^{(1)} \int_{Q_{\min}}^{Q_{\max}} dQ \mathcal{I}_\tau(Q) \frac{1}{Q^3} \alpha^2(Q) H(Q) \right. \\ &\times \int_{e^{y_{\min}}}^{e^{y_{\max}}} d\xi \mathcal{I}_\alpha(\xi) \frac{1}{\xi} \sum_q C_q(Q) \bar{F}_q \left( \frac{Q}{\sqrt{s}} \xi, b_* \left( \frac{z_n}{q_T} \right); Q \right) \bar{F}_{\bar{q}} \left( \frac{Q}{\sqrt{s}} \frac{1}{\xi}, b_* \left( \frac{z_n}{q_T} \right); Q \right) \Big] \\ &\times f_{\text{NP}} \left( \frac{Q_\tau}{\sqrt{s}} \xi_\alpha, \frac{z_n}{q_T}; Q_\tau \right) f_{\text{NP}} \left( \frac{Q_\tau}{\sqrt{s}} \frac{1}{\xi_\alpha}, \frac{z_n}{q_T}; Q_\tau \right).\end{aligned}\quad (42)$$

In conclusion, if we define:

$$\begin{aligned}W_{n\tau\alpha}(q_T) &\equiv w_n^{(1)} \frac{8\pi}{9} \int_{Q_{\min}}^{Q_{\max}} dQ \mathcal{I}_\tau(Q) \frac{\alpha^2(Q)}{Q^3} H(Q) \\ &\times \int_{e^{y_{\min}}}^{e^{y_{\max}}} d\xi \mathcal{I}_\alpha(\xi) \frac{1}{\xi} \sum_q C_q(Q) \bar{F}_q \left( \frac{Q}{\sqrt{s}} \xi, b_* \left( \frac{z_n}{q_T} \right); Q \right) \bar{F}_{\bar{q}} \left( \frac{Q}{\sqrt{s}} \frac{1}{\xi}, b_* \left( \frac{z_n}{q_T} \right); Q \right),\end{aligned}\quad (43)$$

the quantity  $\tilde{K}(q_T)$  can be computed as:

$$\tilde{K}(q_T) \simeq \sum_{n=1}^N \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_\xi} W_{n\tau\alpha}(q_T) f_{\text{NP}} \left( \frac{Q_\tau}{\sqrt{s}} \xi_\alpha, \frac{z_n}{q_T}; Q_\tau \right) f_{\text{NP}} \left( \frac{Q_\tau}{\sqrt{s}} \frac{1}{\xi_\alpha}, \frac{z_n}{q_T}; Q_\tau \right). \quad (44)$$

The advantage of Eq. (44) is that the weights  $W_{n\tau\alpha}$ , that clearly depend on  $q_T$  but also on the intervals  $[Q_{\min} : Q_{\max}]$  and  $[y_{\min} : y_{\max}]$ , can be precomputed once and for all for each of the experimental points included in a fit and used to determine the function  $f_{\text{NP}}$ . This provides a fast tool for the computation of predictions that makes the extraction of the non-perturbative part of the TMDs much easier.

It is now time to discuss how the weights defined in Eq. (43) are affected by the presence of cuts as discussed in Sect. 2.1.1. In principle, the function between square brackets in Eq. (33) should be inside the integrals in Eq. (43) and integrated over the variable  $Q$  and  $\xi = e^y$ . However, this turns out to be numerically problematic because the phase-space-reduction function  $\mathcal{P}$  is expensive to compute. On top of this, the fact that the factor between square brackets in Eq. (33) depends on whether  $q_T$  is a lower or an upper integration bound would lead to a duplication of the weights to compute. In order to simplify the computation, we assume that the function  $\mathcal{P}$  and its derivative  $\mathcal{P}'$  are slowly varying functions of  $Q$  and  $y$  over the typical grid interval of the grids in  $Q$  and  $\xi$ . In addition, the interpolating functions  $\mathcal{I}_\tau(Q)$  and  $\mathcal{I}_\alpha(\xi)$  are strongly peaked at  $Q_\tau$  and  $\xi_\alpha$ , respectively. These considerations allow us to avoid integrating explicitly  $\mathcal{P}$  and  $\mathcal{P}'$  over  $Q$  and  $\xi$  and to replace the weights in Eq. (43) with:

$$W_{n\tau\alpha}(q_T) \rightarrow [\mathcal{P}(Q_\tau, \ln(\xi_\alpha), q_T) \pm \mathcal{P}'(Q_\tau, \ln(\xi_\alpha), q_T) \Delta q_T] W_{n\tau\alpha}(q_T). \quad (45)$$

At the end of the day, the only additional information required to implement cuts on the final state is the value of the phase-space-reduction function  $\mathcal{P}$  and its derivative  $\mathcal{P}'$  on all points of the bidimensional grid in  $Q$  and  $\xi$  for all  $q_T$  bin bounds. Eq. (45) will then allow one to use the weights computed over the full phase space. We will check the accuracy of this procedure by comparing it to the explicit integration.

## 2.4 Cross section differential in $x_F$

In some cases, the Drell-Yan differential cross section may be presented as differential in the invariant mass of the lepton pair  $Q$  and, instead of the rapidity  $y$ , of the Feynman variable  $x_F$  defined as:

$$x_F = \frac{Q}{\sqrt{s}} (e^y - e^{-y}) = \frac{2Q}{\sqrt{s}} \sinh y = x_1 - x_2, \quad (46)$$

so that:

$$\frac{dx_F}{dy} = \frac{2Q}{\sqrt{s}} \cosh y = x_1 + x_2. \quad (47)$$

Therefore:

$$\frac{d\sigma}{dQ dx_F dq_T} = \frac{dy}{dx_F} \frac{d\sigma}{dQ dy dq_T} = \frac{\sqrt{s}}{2Q \cosh y} \frac{d\sigma}{dQ dy dq_T} = \frac{1}{x_1 + x_2} \frac{d\sigma}{dQ dy dq_T} \quad (48)$$

with:

$$y(x_F, Q) = \sinh^{-1} \left( \frac{x_F \sqrt{s}}{2Q} \right) = \ln \left[ \frac{\sqrt{s}}{2Q} \left( x_F + \sqrt{x_F^2 + \frac{4Q^2}{s}} \right) \right], \quad (49)$$

so that:

$$x_1 = \frac{1}{2} \left( x_F + \sqrt{x_F^2 + \frac{4Q^2}{s}} \right) \quad \text{and} \quad x_2 = \frac{Q^2}{sx_1}. \quad (50)$$

Therefore, we can compute the integral:

$$\tilde{I}(q_T) = \int_{Q_{\min}}^{Q_{\max}} dQ \int_{x_{F,\min}}^{x_{F,\max}} dx_F I(Q, x_F, q_T), \quad (51)$$

where  $I$  is the primitive in  $q_T$  of the cross section differential in  $x_F$ :

$$I(Q, x_F, q_T) = \int dq_T \left[ \frac{d\sigma}{dQ dx_F dq_T} \right], \quad (52)$$

following the same steps of Sect. 2.3. This leads to:

$$\tilde{I}(q_T) \simeq \sum_{n=1}^N \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_x} \bar{W}_{n\tau\alpha}(q_T) f_{\text{NP}} \left( x_{1,\alpha\tau}, \frac{z_n}{q_T}; Q_\tau \right) f_{\text{NP}} \left( x_{2,\alpha\tau}, \frac{z_n}{q_T}; Q_\tau \right), \quad (53)$$

with:

$$\begin{aligned} \bar{W}_{n\tau\alpha}(q_T) &\equiv w_n^{(1)} \frac{8\pi}{9} \int_{Q_{\min}}^{Q_{\max}} dQ \mathcal{I}_\tau(Q) \frac{1}{Q^3} \alpha^2(Q) H(Q) \\ &\times \int_{x_{F,\min}}^{x_{F,\max}} dx_F \mathcal{I}_\alpha(x_F) \frac{1}{x_1 + x_2} \sum_q C_q(Q) \bar{F}_q \left( x_1, b_* \left( \frac{z_n}{q_T} \right); Q \right) \bar{F}_{\bar{q}} \left( x_2, b_* \left( \frac{z_n}{q_T} \right); Q \right), \end{aligned} \quad (54)$$

where  $x_1$  and  $x_2$  are functions of  $x_F$  and  $Q$  through Eq. (50). In addition, we have defined a grid in  $x_F$ ,  $\{x_{F,\alpha}\}$  with  $\alpha = 0, \dots, N_x$ , that allowed us to define  $x_{1(2),\alpha\tau} \equiv x_{1(2)}(x_{F,\alpha}, Q_\tau)$ .

## 2.5 Flavour dependence

It may be advantageous to introduce a flavour dependence of the non-perturbative contributions to TMDs. This can be easily done by observing that the tensor  $W_{n\tau\alpha}$  defined in Eq. (43) can be decomposed as<sup>5</sup>:

$$W_{n\tau\alpha}(q_T) = \sum_q W_{n\tau\alpha}^{(q)}(q_T), \quad (55)$$

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<sup>5</sup>The same procedure applies to the tensor  $\bar{W}_{n\tau\alpha}$  defined in Eq. (54).



with:

$$\begin{aligned}
W_{n\tau\alpha}^{(q)}(q_T) &\equiv w_n^{(1)} \frac{8\pi}{9} \int_{Q_{\min}}^{Q_{\max}} dQ \mathcal{I}_\tau(Q) \frac{\alpha^2(Q)}{Q^3} H(Q) C_q(Q) \\
&\times \int_{e^{y_{\min}}}^{e^{y_{\max}}} d\xi \mathcal{I}_\alpha(\xi) \frac{1}{\xi} \bar{F}_q \left( \frac{Q}{\sqrt{s}} \xi, b_* \left( \frac{z_n}{q_T} \right); Q \right) \bar{F}_{\bar{q}} \left( \frac{Q}{\sqrt{s}} \frac{1}{\xi}, b_* \left( \frac{z_n}{q_T} \right); Q \right).
\end{aligned} \tag{56}$$

This allows for an independent parameterisation of the non-perturbative contribution such that Eq. (44) can be written as:

$$\tilde{K}(q_T) \simeq \sum_q \sum_{n=1}^N \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_\xi} W_{n\tau\alpha}^{(q)}(q_T) f_{\text{NP}}^{(q)} \left( \frac{Q_\tau}{\sqrt{s}} \xi_\alpha, \frac{z_n}{q_T}; Q_\tau \right) f_{\text{NP}}^{(q)} \left( \frac{Q_\tau}{\sqrt{s}} \frac{1}{\xi_\alpha}, \frac{z_n}{q_T}; Q_\tau \right), \tag{57}$$

where  $f_{\text{NP}}^{(q)}$  parametrises the non-perturbative component of the TMD with flavour  $q$ .

## 2.6 Gradient with respect to the free parameters

A very appealing implication of the computation of cross section in terms of precomputed table as in Eqs. (44) and (57) is the fact that it exposes the free parameters of the non-perturbative functions. To be more specific, the non-perturbative function  $f_{\text{NP}}$ , on top of being a function of  $x$ ,  $b$ , and  $\zeta$ , depends parameterically on a set of  $N_p$  parameters  $\{\theta_k\}$ ,  $k = 1, \dots, N_p$ , that are typically determined by fits to data, in other words:

$$f_{\text{NP}} \equiv f_{\text{NP}}(x, b, \zeta; \{\theta_k\}). \tag{58}$$

Now, when performing a fit, it is very useful to be able to compute the derivative of the figure of merit (usually the  $\chi^2$ ) with respect to the parameters to be determined. In turn, this immediately implies being able to compute the derivative of the observables. Referring to Eq. (44), the relevant quantity is:

$$\frac{d\tilde{K}}{d\theta_k} = \sum_{n=1}^N \sum_{\tau=0}^{N_Q} \sum_{\alpha=0}^{N_\xi} W_{n\tau\alpha}(q_T) \left[ \frac{df_{\text{NP}}^{(1)}}{d\theta_k} f_{\text{NP}}^{(2)} + f_{\text{NP}}^{(1)} \frac{df_{\text{NP}}^{(2)}}{d\theta_k} \right], \tag{59}$$

where  $f_{\text{NP}}^{(1)}$  and  $f_{\text{NP}}^{(2)}$  refer to the non-perturbative function  $f_{\text{NP}}$  computed in  $x_1$  and  $x_2$ , respectively. It is thus clear that the derivatives w.r.t. the free parameters penetrates the observable. Since in most cases the derivative of  $f_{\text{NP}}$  can be computed analytically, this allows one to compute the gradient of the figure of merit analytically. This potentially makes any fit much simpler.

## 2.7 Narrow-width approximation

A possible alternative to the numerical integration in  $Q$  when the integration region includes the  $Z$ -peak region is the so-called narrow-width approximation (NWA). In the NWA one assumes that the width of the  $Z$  boson,  $\Gamma_Z$ , is much smaller than its mass,  $M_Z$ . This way one can approximate the peaked behaviour of the couplings  $C_q(Q)$  around  $Q = M_Z$  with a  $\delta$ -function, *i.e.*  $C_q(Q) \sim \delta(Q^2 - M_Z^2)$ . Therefore, the integration over  $Q$  can be done analytically. The exact structure of the electroweak couplings is the following:

$$C_q(Q) = e_q^2 - 2e_q V_q V_e \chi_1(Q) + (V_e^2 + A_e^2)(V_q^2 + A_q^2) \chi_2(Q), \tag{60}$$

with:

$$\begin{aligned}
\chi_1(Q) &= \frac{1}{4 \sin^2 \theta_W \cos^2 \theta_W} \frac{Q^2(Q^2 - M_Z^2)}{(Q^2 - M_Z^2)^2 + M_Z^2 \Gamma_Z^2}, \\
\chi_2(Q) &= \frac{1}{16 \sin^4 \theta_W \cos^4 \theta_W} \frac{Q^4}{(Q^2 - M_Z^2)^2 + M_Z^2 \Gamma_Z^2}.
\end{aligned} \tag{61}$$

In the limit  $\Gamma_Z/M_Z \rightarrow 0$ , the leading contribution to the coupling in Eq. (60) comes from the region  $Q \simeq M_Z$  and is that proportional to  $\chi_2$ :

$$C_q(Q) \simeq (V_e^2 + A_e^2)(V_q^2 + A_q^2)\chi_2(Q), \quad Q \simeq M_Z. \quad (62)$$

In addition, in this limit one can show that:

$$\frac{1}{(Q^2 - M_Z^2)^2 + M_Z^2 \Gamma_Z^2} \rightarrow \frac{\pi}{M_Z \Gamma_Z} \delta(Q^2 - M_Z^2) = \frac{\pi}{2M_Z^2 \Gamma_Z} \delta(Q - M_Z). \quad (63)$$

Therefore, considering that:

$$\Gamma_Z = \frac{\alpha M_Z}{\sin^2 \theta_W \cos^2 \theta_W}, \quad (64)$$

the electroweak couplings in the NWA have the following form:

$$C_q(Q) \simeq \frac{\pi M_Z (V_e^2 + A_e^2)(V_q^2 + A_q^2)}{32\alpha \sin^2 \theta_W \cos^2 \theta_W} \delta(Q - M_Z) = \tilde{C}_q(Q) \delta(Q - M_Z). \quad (65)$$

Therefore, using Eq. (65) the integral of the cross section over  $Q$  under the condition that  $Q_{\min} < M_Z < Q_{\max}$  has the consequence of adjusting the couplings and of setting  $Q = M_Z$  in the computation. This yields:

$$\int_{Q_{\min}}^{Q_{\max}} dQ \frac{d\sigma}{dQ dy dq_T} = \frac{16\pi\alpha^2 q_T}{9M_Z^3} H(M_Z, M_Z) \sum_q \tilde{C}_q(M_Z) I_{q\bar{q}}(x_1, x_2, q_T; M_Z, M_Z^2), \quad (66)$$

where we are also assuming that  $\mu = \sqrt{\zeta} = M_Z$ . As a final step, one may want to let the  $Z$  boson decay into leptons. At leading order in the EW sector and assuming an equal decay rate for electrons, muons, and tauons, this can be done by multiplying the cross section above by three times the branching ratio for the  $Z$  decaying into any pair of leptons,  $3\text{Br}(Z \rightarrow \ell^+ \ell^-)$ .

## A Ogata quadrature

In this section we limit ourselves to write the formulas for the computation of the unscaled coordinates  $z_n^{(\nu)}$  and weights  $w_n^{(\nu)}$  required to compute the following integral:

$$I_\nu(q_T) = \int_0^\infty db J_\nu(bq_T) f(b) = \frac{1}{q_T} \int_0^\infty d\bar{b} J_\nu(\bar{b}) f\left(\frac{\bar{b}}{q_T}\right) \simeq \frac{1}{q_T} \sum_{n=1}^\infty w_n^{(\nu)} f\left(\frac{z_n^{(\nu)}}{q_T}\right) \quad \nu = 0, 1, \dots, \quad (67)$$

using the Ogata-quadrature algorithm. More details can be found in Ref. [3]. There relevant formulas are:

$$z_n^{(\nu)} = \frac{\pi}{h} \psi\left(\frac{h\xi_{\nu n}}{\pi}\right), \quad (68)$$

$$w_n^{(\nu)} = \pi \frac{Y_\nu(\xi_{\nu n})}{J_{\nu+1}(\xi_{\nu n})} J_\nu(z_n^{(\nu)}) \psi'\left(\frac{h\xi_{\nu n}}{\pi}\right).$$

where:

- $h$  is a free parameter of the algorithm that has to be typically small (we choose  $h = 10^{-3}$ ),
- $\xi_{\nu n}$  are the zero's of  $J_\nu$ , *i.e.*  $J_\nu(\xi_{\nu n}) = 0 \forall n$ ,
- $J_\nu$  and  $Y_\nu$  are the Bessel functions of first and second kind, respectively, of degree  $\nu$ ,
- $\psi$  is the following function:

$$\psi(t) = t \tanh\left(\frac{\pi}{2} \sinh t\right) \quad (69)$$

and its derivative:

$$\psi'(t) = \frac{\pi t \cosh t + \sinh(\pi \sinh t)}{1 + \cosh(\pi \sinh t)}. \quad (70)$$

## B Lagrange interpolation

Just for the record, it is useful to derive a general expression for the Lagrange interpolating functions  $\mathcal{I}$  introduced in Eq. (40) and used to interpolate the non-perturbative functions  $f_{\text{NP}}$ . More, importantly, we need to understand how these functions behave upon integration.

Suppose one wants to interpolate the test function  $g$  in the point  $x$  using a set of Lagrange polynomials of degree  $k$  of. This requires a subset of  $k+1$  consecutive points on an interpolation grid, say  $\{x_\alpha, \dots, x_{\alpha+k}\}$ . The relative position between the point  $x$  and the subset of points used for the interpolation is arbitrary. It is convenient to choose the subset of points such that  $x_\alpha < x \leq x_{\alpha+k}$ .<sup>6</sup> However, the ambiguity remains because there are  $k$  possible choices according to whether  $x_\alpha < x \leq x_{\alpha+1}$ , or  $x_{\alpha+1} < x \leq x_{\alpha+2}$ , and so on.

In order to determine the exact form of the interpolation functions  $\mathcal{I}$ , let us see how to derive eq. (40). Using the standard Lagrange interpolation procedure, we can approximate the function  $g$  in  $x$  as:

$$g(x) = \sum_{i=0}^k \ell_i^{(k)}(x) g(x_{\alpha+i}), \quad (71)$$

where  $\ell_i^{(k)}$  is the  $i$ -th Lagrange polynomial of degree  $k$  which can be written as:

$$\ell_i^{(k)}(x) = \prod_{m=0, m \neq i}^k \frac{x - x_{\alpha+m}}{x_{\alpha+i} - x_{\alpha+m}}. \quad (72)$$

We now assume that:

$$x_\alpha < x \leq x_{\alpha+1}, \quad (73)$$

Eq. (71) becomes:

$$g(x) = \theta(x - x_\alpha) \theta(x_{\alpha+1} - x) \sum_{i=0}^k g(x_{\alpha+i}) \prod_{m=0, m \neq i}^k \frac{x - x_{\alpha+m}}{x_{\alpha+i} - x_{\alpha+m}}. \quad (74)$$

In order to make Eq. (74) valid for all values of  $\alpha$ , one just has to sum over all  $N_x$  intervals of the *global* interpolation grid  $\{x_0, \dots, x_{N_x}\}$ , that is:

$$g(x) = \sum_{\alpha=0}^{N_x-1} \theta(x - x_\alpha) \theta(x_{\alpha+1} - x) \sum_{i=0}^k g(x_{\alpha+i}) \prod_{m=0, m \neq i}^k \frac{x - x_{\alpha+m}}{x_{\alpha+i} - x_{\alpha+m}}, \quad (75)$$

Defining  $\beta = \alpha + i$ , we can rearrange the equation above as:

$$g(x) = \sum_{\beta=0}^{N_x+k-1} \mathcal{I}_\beta^{(k)}(x) g(x_\beta), \quad (76)$$

that leads us to the definition of the interpolating functions:

$$\mathcal{I}_\beta^{(k)}(x) = \sum_{i=0, i \leq \beta}^k \theta(x - x_{\beta-i}) \theta(x_{\beta-i+1} - x) \prod_{m=0, m \neq i}^k \frac{x - x_{\beta-i+m}}{x_\beta - x_{\beta-i+m}}, \quad (77)$$

where the condition  $i \leq \beta$  comes from the condition  $\alpha \geq 0$ . It is important to observe that the sum in Eq. (76) extends up to the  $(N_x + k - 1)$ -th node. Therefore, the original grid needs to be extended by  $k - 1$  nodes. However, the range of validity of the interpolation remains that defined by the original

<sup>6</sup>In fact, it is not even necessary to impose the constraint  $x_\alpha < x \leq x_{\alpha+k}$ . In case this relation is not fulfilled one usually refers to *extrapolation* rather than *interpolation*. If not necessary, this option is typically not convenient because it may lead to a substantial deterioration in the accuracy with which  $g(x)$  is determined.

grid, *i.e.*  $x_0 \leq x \leq x_{N_x}$ . Finally, it is crucial to realise that the interpolation function  $\mathcal{I}_\beta^{(k)}(x)$  is different from zero only over a limited interval, specifically:

$$\mathcal{I}_\beta^{(k)}(x) \neq 0 \quad \Leftrightarrow \quad x_{\beta-k} < x < x_{\beta+1}. \quad (78)$$

In the rest of this document we will stick to the assumption in Eq. (73). However, before going further, it is interesting to generalise Eq. (73) to:

$$x_{\alpha+t} < x \leq x_{\alpha+t+1} \quad \text{with} \quad t = 0, \dots, k-1, \quad (79)$$

such that the interpolation formula becomes:

$$g(x) = \sum_{\alpha=-t}^{N_x-t-1} \theta(x - x_{\alpha+t}) \theta(x_{\alpha+t+1} - x) \sum_{i=0}^k g(x_{\alpha+i}) \prod_{m=0, m \neq i}^k \frac{x - x_{\alpha+m}}{x_{\alpha+i} - x_{\alpha+m}}, \quad (80)$$

that can be rearranged as:

$$g(x) = \sum_{\beta=-t}^{N_x+k-t-1} \mathcal{I}_{\beta,t}^{(k)}(x) g(x_\beta), \quad (81)$$

with:

$$\mathcal{I}_{\beta,t}^{(k)}(x) = \sum_{i=0, i \leq \beta}^k \theta(x - x_{\beta-i+t}) \theta(x_{\beta-i+t+1} - x) \prod_{m=0, m \neq i}^k \frac{x - x_{\beta-i+m}}{x_\beta - x_{\beta-i+m}}, \quad (82)$$

being the “generalised” interpolation functions. The generalised interpolation functions can be used to overcome the “drawback” of requiring  $k-1$  additional nodes on the interpolation grid. In practice, given the grid  $\{x_0, \dots, x_{N_x}\}$ , one can tune  $t$  according to the position of  $x$  on the grid. More specifically, one can choose  $t$  in such a way that  $\beta+t$  in Eq. (82) never exceeds  $N_x$ .

Now suppose we want to compute the following integral:

$$I_1 = \int_{x_0}^{x_{N_x}} dx g(x) f(x), \quad (83)$$

where  $f$  is some other function that we don’t want to interpolate. Using Eqs. (76) and (78) we finally have that:

$$I_1 = \sum_{\beta=0}^{N_x+k-1} W_\beta g(x_\beta), \quad (84)$$

with:

$$W_\beta = \int_{x_{\max(0, \beta-k)}}^{x_{\min(N_x, \beta+1)}} dx \mathcal{I}_\beta^{(k)}(x) f(x). \quad (85)$$

The equation above can be easily generalised to a bidimensional integral as:

$$I_2 = \int_{x_0}^{x_{N_x}} dx \int_{y_0}^{y_{N_y}} dy g(x, y) f(x, y) = \sum_{\alpha=0}^{N_x+k-1} \sum_{\beta=0}^{N_y+l-1} W_{\alpha\beta} g(x_\alpha, y_\beta), \quad (86)$$

with:

$$W_{\alpha\beta} = \int_{x_{\max(0, \alpha-k)}}^{x_{\min(N_x, \alpha+1)}} dx \int_{y_{\max(0, \beta-k)}}^{y_{\min(N_y, \beta+1)}} dy \mathcal{I}_\alpha^{(k)}(x) \mathcal{I}_\beta^{(l)}(y) f(x, y). \quad (87)$$

This formalism nicely applies to the integral in  $Q$  and  $\xi = e^y$  discussed above in Eq. (43). In view of a numerical implementation, it is worth noticing that the functions  $\mathcal{I}$  are piecewise. In particular, while these functions are continuous in correspondence of the nodes of the grid, their first derivative is not. As a consequence, the result of the numerical integrals in Eqs. (85) and (87) may be inaccurate. To overcome this problem, it is sufficient to split the integrals in sub-integrals over the intervals delimited by two consecutive nodes. Using Eq. (78), it is easy to see that, for an interpolation of degree  $k$ , one needs to do  $k+1$  integrals over the intervals included between the  $(\beta-k)$ -th and the  $(\beta+1)$ -th node.

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