Generating functions, Mellin transformations and twist-2 operator matrix elements in QCD

Arnd Behring

CERN
Theory Department

based on [arXiv:2211.05462], [arXiv:2303.05943], [arXiv:2311.00644]
in collaboration with J. Ablinger, J. Blümlein, A. De Freitas, A. Goedicke, C. Schneider, K. Schönwald, A. von Manteuffel

December 15, 2023 – QCD Meets Gravity 2023 – CERN

Motivation: Variable flavour number scheme for PDFs

Example:
LHC processes involving b quarks

massless u, d, s, c and massive b

- u, d, s, c PDFs
- b only produced perturbatively
- potentially large $\ln(Q^2/m_b^2)$

massless u, d, s, c and b

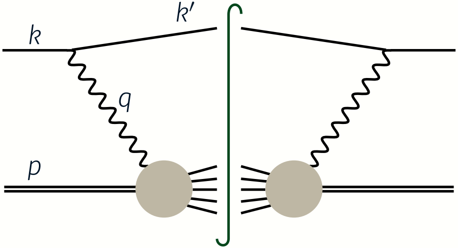
- u, d, s, c and b PDFs
- DGLAP equations resum collinear singularities

- Appropriate description depends on relevant scales of the process
- Match PDFs in both schemes at a matching scale, e.g.,

$$f_Q(n_f+1) + f_{\bar{Q}}(n_f+1) = \mathbf{A}_{\mathbf{Qq}}^{\mathbf{PS}} \otimes \sum_k [f_k(n_f) + f_{\bar{k}}(n_f)] + \mathbf{A}_{\mathbf{Qg}} \otimes G(n_f)$$

→ Knowing the matching coefficients A_{ij} (massive operator matrix elements (OMEs)) at $\mathcal{O}(\alpha_s^3)$ is important, e.g., for precision PDFs

Motivation: Deep-inelastic scattering



$\rightsquigarrow$ Leptonic tensor $L_{\mu\nu}$

$\rightsquigarrow$ Hadronic tensor $W^{\mu\nu}$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}x\,\mathrm{d}Q^2} = \frac{2\pi\alpha^2}{xQ^4} L_{\mu\nu} W^{\mu\nu}$$

$$Q^2 = -q^2, x = \frac{Q^2}{2\,p\cdot q}$$

Hadronic tensor can be decomposed into structure functions:

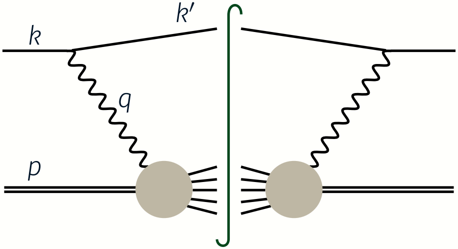
$$W^{\mu\nu} = (\dots)^{\mu\nu} F_2(x, Q^2) + (\dots)^{\mu\nu} F_L(x, Q^2)$$

$$\hookrightarrow F_2(x, Q^2) = x \sum_i \mathcal{C}_{2,i} \otimes f_i$$

Wilson coefficients ($\mathcal{C}_{2,i}$)

parton distribution functions (PDFs) (f_i)

Motivation: Deep-inelastic scattering



$\rightsquigarrow$ Leptonic tensor $L_{\mu\nu}$

$\rightsquigarrow$ Hadronic tensor $W^{\mu\nu}$

$$\frac{d\sigma}{dx\, dQ^2} = \frac{2\pi\alpha^2}{xQ^4} L_{\mu\nu} W^{\mu\nu}$$

$$Q^2 = -q^2,\; x = \frac{Q^2}{2\, p \cdot q}$$

Hadronic tensor can be decomposed into structure functions:

$$W^{\mu\nu} = (\dots)^{\mu\nu} F_2(x, Q^2) + (\dots)^{\mu\nu} F_L(x, Q^2)$$

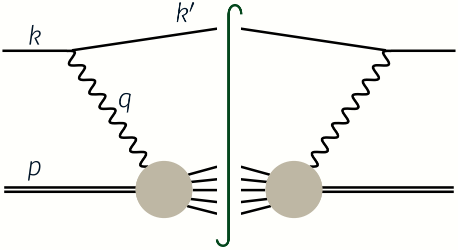
$$\hookrightarrow F_2(x, Q^2) = x \sum_i \mathcal{C}_{2,i} \otimes f_i$$

massless [Moch et al. '05] [Blümlein et al. '22]

massive

$$\hookrightarrow \mathcal{C}_{2,i} = C_{2,i} + H_{2,i} = \sum_j C_{2,j} \otimes \mathrm{A}_{ji} + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

Motivation: Deep-inelastic scattering



$\rightsquigarrow$ Leptonic tensor $L_{\mu\nu}$

$\rightsquigarrow$ Hadronic tensor $W^{\mu\nu}$

$$\frac{d\sigma}{dx\, dQ^2} = \frac{2\pi\alpha^2}{xQ^4} L_{\mu\nu} W^{\mu\nu}$$

$$Q^2 = -q^2,\ x = \frac{Q^2}{2\, p \cdot q}$$

Hadronic tensor can be decomposed into structure functions:

$$W^{\mu\nu} = (\dots)^{\mu\nu} F_2(x, Q^2) + (\dots)^{\mu\nu} F_L(x, Q^2)$$

$$\hookrightarrow F_2(x, Q^2) = x \sum_i \mathcal{C}_{2,i} \otimes f_i$$

massless [Moch et al. ’05] [Blümlein et al. ’22]

massive

$$\hookrightarrow \mathcal{C}_{2,i} = C_{2,i} + H_{2,i} = \sum_j C_{2,j} \otimes \mathrm{A}_{ji} + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

Heavy flavour contribution factorises for $Q^2 \gg m^2$ into massless Wilson coefficients and massive operator matrix elements [Buza, Matiounine, Smith, van Neerven ’96]

$\rightarrow$ Knowing the OMEs to $\mathcal{O}(\alpha_s^3)$ is important for precise description of DIS.

x and N space: Mellin transformations

Two equivalent formulations of the problem in x space and Mellin N space

$$F_2(x, Q^2) = x \sum_i \mathcal{C}_{2,i} \otimes f_i$$

$$[f \otimes g](x) = \int_x^1 \mathrm{d}z\, f(z) g\left(\frac{x}{z}\right)$$

Mellin transformation

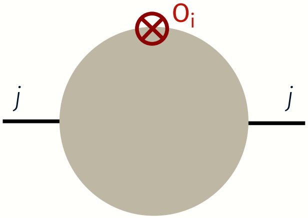
$$\tilde{f}(N) = \int_0^1 \mathrm{d}x^{N-1} f(x)$$

$$[f \otimes g](N) = \tilde{f}(N)\tilde{g}(N)$$

Calculating operator matrix elements

Goal: Calculate massive operator matrix elements A_{ij} at $\mathcal{O}(\alpha_s^3)$

Definition:



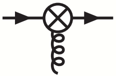
$$A_{ij}(N) = \Delta_{\mu_1} \dots \Delta_{\mu_N} \langle j | O_i^{\mu_1 \dots \mu_N} | j \rangle \qquad \Delta^2 = 0$$

$$O_q^{\mu_1 \dots \mu_N} = \mathrm{i}^{N-1} \mathbf{S} \left[\bar{\psi} \gamma^{\mu_1} D^{\mu_2} \dots D^{\mu_N} \psi \right] - \text{trace terms}$$

$$O_g^{\mu_1 \dots \mu_N} = 2\mathrm{i}^{N-2} \mathbf{S}\, \mathrm{Tr} \left[G^{a,\mu_1}{}_{\alpha} D^{\mu_2} \dots D^{\mu_{N-1}} G_a^{\alpha \mu_N} \right] - \text{trace terms}$$

Feynman rules for operator insertions:

p  p $\quad \sim (\Delta \cdot p)^{N-1}$

p_1  p_2 $\quad \sim \sum_{j=0}^{N-2} (\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-j-2}$

Problem: Need results for general N

$\rightarrow$ How to do IBP reductions for arbitrary rank tensor integrals?

Generating functions

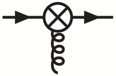
Idea: Introduce generating function for Mellin moments [Ablinger et al. '12]

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \tilde{f}(N)$$

Apply to tensor integrals:

p  p

$$\rightarrow \sum_{N=1}^{\infty} t^N (\Delta \cdot p)^{N-1} = \frac{t}{1 - t(\Delta \cdot p)}$$

p_1  p_2

$$\rightarrow \sum_{N=1}^{\infty} t^N \sum_{j=0}^{N-2} (\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-j-2} = \frac{t^2}{[1 - t(\Delta \cdot p_1)][1 - t(\Delta \cdot p_2)]}$$

- Can apply IBP reductions with linear propagators
- Expansion coefficients around $t = 0$ are Mellin moments

Computational workflow so far

N space

- Generate diagrams & insert Feynman rules
- Simplify Dirac, Lorentz and colour algebra

t space

- Map integrals to integral families
- IBP reduction to master integrals (MIs)
- Derive differential equations for MIs

N space

- Translate to difference equations for MIs
- Solve MIs in *N* space
- Assemble *N* space result

x space

- Translate final result from *N* to *x* space

Build on powerful toolbox for summation in difference fields, handling nested sums and iterated integrals, etc.
`Sigma`, `HarmonicSums`, `EvaluateMultiSums`, `OreSys`, `SumProduction`, `SolveCoupledSystem`, ...

Expected function classes

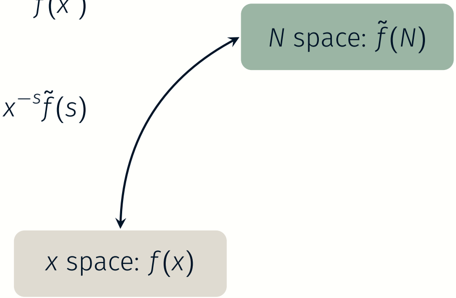
Sums	(Inv.) Mellin transformation	Integrals	
Harmonic sums $\sum_{i=1}^{N}\frac{1}{i}\sum_{j=1}^{i}\frac{(-1)^j}{j^2}$	⟷	Harmonic polylogarithms $\int_0^x\frac{dy}{1-y}\int_0^y\frac{dz}{1+z}$	First-order factorisable diff. equations
Generalised harm. sums $\sum_{i=1}^{N}\frac{2^i}{i}\sum_{j=1}^{i}\frac{2^{-j}}{j^2}$	⟷	Generalised HPLs $\int_0^x\frac{dy}{\frac{1}{2}-y}\int_0^y\frac{dz}{2-z}$	First-order factorisable diff. equations
Cyclotomic harm. sums $\sum_{i=1}^{N}\frac{1}{3i+2}\sum_{j=1}^{i}\frac{1}{3j+1}$	⟷	Cyclotomic HPLs $\int_0^x\frac{dy}{1-y}\int_0^y\frac{dz}{1+z+z^2}$	First-order factorisable diff. equations
Binomial sums $\sum_{i=1}^{N}\frac{1}{\binom{2i}{i}i}\sum_{j=1}^{i}\binom{2j}{j}$	⟷	Root-valued letters $\int_0^x\frac{dy}{1-y}\int_0^y\frac{dz}{\sqrt{z(4-z)}}$	First-order factorisable diff. equations
?	⟷	Transcendental kernels $\int_0^x dz\, {}_2F_1\left[\begin{matrix}\frac{4}{3},\frac{5}{3}\\ 2\end{matrix};\frac{z^2(z^2-9)^2}{(z^2+3)^3}\right]$	Non-first-order factorisable diff. equations

x space, N space and t space

Mellin transformation:

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x'\, x'^{N-1} f(x')$$

$$f(x) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}s\, x^{-s} \tilde{f}(s)$$



x space, N space and t space

Mellin transformation:

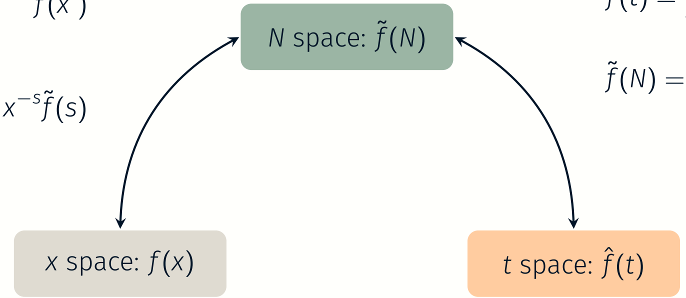
$$\tilde{f}(N) = \int_0^1 \mathrm{d}x'\, x'^{N-1} f(x')$$

$$f(x) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}s\, x^{-s} \tilde{f}(s)$$

Generating function:

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \tilde{f}(N)$$

$$\tilde{f}(N) = [t^N]\,\hat{f}(t)$$



x space, N space and t space

Mellin transformation:

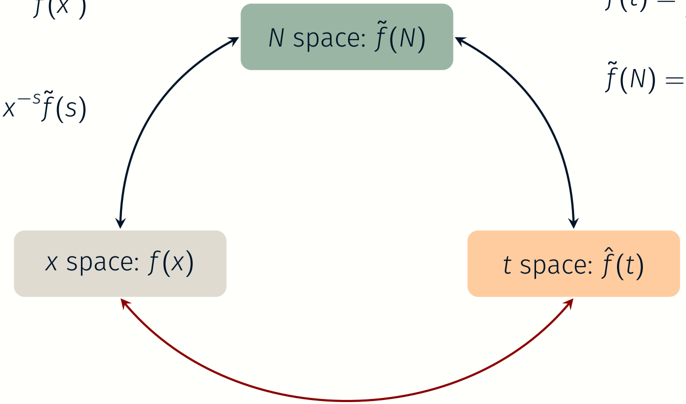
$$\tilde{f}(N) = \int_0^1 \mathrm{d}x' \, x'^{N-1} f(x')$$

$$f(x) = \frac{1}{2\pi \mathrm{i}} \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}s \, x^{-s} \tilde{f}(s)$$

Generating function:

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \tilde{f}(N)$$

$$\tilde{f}(N) = [t^N] \hat{f}(t)$$



Can we find the x space expression directly from t space?

$\rightarrow$ Yes! [AB, Blümlein, Schönwald '23]

From t- to x-space: Derivation (regular case)

$$f(x)$$

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x' \, x'^{N-1} f(x')$$

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \tilde{f}(N)$$

From t- to x-space: Derivation (regular case)

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x' \, x'^{N-1} f(x')$$

$$f(x)$$

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \int_0^1 \mathrm{d}x' \, x'^{N-1} f(x')$$

From t- to x-space: Derivation (regular case)

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x'\, x'^{N-1} f(x')$$

$$f(x)$$

$$\hat{f}(t) = \int_0^1 \mathrm{d}x' \frac{t}{1 - tx'} f(x')$$

From t- to x-space: Derivation (regular case)

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x' \, x'^{N-1} f(x')$$

$$f(x)$$

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{1}{x - x'} f(x')$$

From t- to x-space: Derivation (regular case)

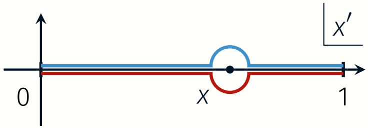
$$\tilde{f}(N) = \int_0^1 \mathrm{d}x'\, x'^{N-1} f(x')$$

$$f(x)$$

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{1}{x - x'} f(x')$$

Sochocki's formula:

$$\lim_{\delta \to 0^+} \frac{1}{\xi \pm \mathrm{i}\delta} = \mathcal{P}\frac{1}{\xi} \mp \mathrm{i}\pi\delta(\xi)$$



From t- to x-space: Derivation (regular case)

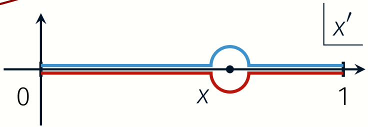
$$\tilde{f}(N) = \int_0^1 \mathrm{d}x'\, x'^{N-1} f(x')$$

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{1}{x - x'} f(x')$$

$$f(x) = \frac{-1}{2\pi \mathrm{i}} \operatorname*{Disc}_x \hat{f}\left(\frac{1}{x}\right)$$

Sochocki's formula:

$$\lim_{\delta \to 0^+} \frac{1}{\xi \pm \mathrm{i}\delta} = \mathcal{P}\frac{1}{\xi} \mp \mathrm{i}\pi\delta(\xi)$$

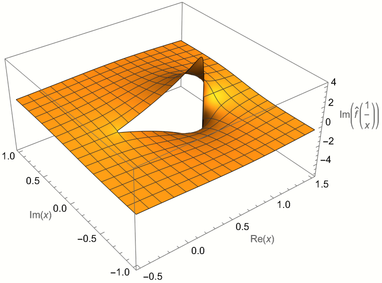


$$\tilde{f}(N) = -\frac{S_1(N)}{N^2} + \frac{\zeta_2}{N}$$

$$f(x) = -H_{0,1}(x)$$

$$\hat{f}(t) = H_{0,0,1}(t) + H_{0,1,1}(t) - \zeta_2 H_1(t)$$

$$f(x) = \frac{-1}{2\pi \mathrm{i}} \operatorname*{Disc}_x \hat{f}\left(\frac{1}{x}\right)$$



$$\hat{f}\left(\frac{1}{x}\right) = -H_{0,1,1}(x) - H_{0,1,0}(x) - \zeta_2 H_1(x) + \zeta_3$$
$$+ \operatorname{sign}(\operatorname{Im}(x))\mathrm{i}\pi H_{0,1}(x)$$

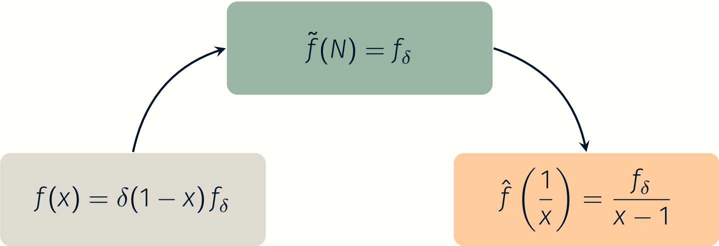
Generalisation: Dealing with $\delta(1-x)$ distributions

$$\tilde{f}(N) = f_\delta$$

$$f(x) = \delta(1-x)\, f_\delta$$

$$\hat{f}(t) = \frac{t\, f_\delta}{1-t}$$

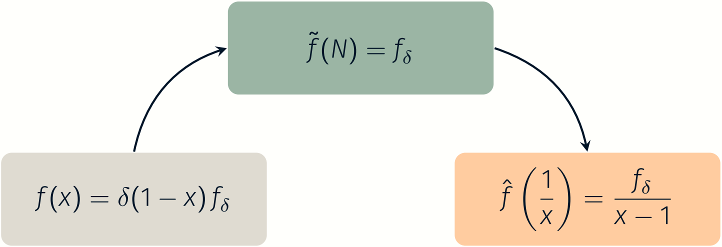
Generalisation: Dealing with $\delta(1-x)$ distributions



- Extract f_δ: Take residue at $x = 1$?

$$f_\delta \stackrel{?}{=} \operatorname*{Res}_{x=1} \hat{f}\left(\frac{1}{x}\right)$$

Generalisation: Dealing with $\delta(1-x)$ distributions



- Extract f_δ: Take residue at $x = 1$?

$$f_\delta \stackrel{?}{=} \operatorname*{Res}_{x=1} \hat{f}\left(\frac{1}{x}\right)$$

- Yes, but: Overlap with branch cuts from regular part must be subtracted first
- Equivalent: Obtain f_δ from $\frac{1}{x-1}$ expansion coefficient of $\hat{f}\left(\frac{1}{x}\right)$

Generalisation: Dealing with plus distributions

$$f(x) = f_{+,k}\left[\frac{\ln^k(1-x)}{1-x}\right]_+$$

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x\,(x^{N-1}-1) f_{+,k}\frac{\ln^k(1-x)}{1-x} = -f_{+,k}\,k!\,S_{\underbrace{1,\ldots,1}_{k \text{ times}}}(N-1)$$

$$\hat{f}(t) \sim \frac{f_{+,k}}{k+1}\frac{\ln^{k+1}(1-t)}{t-1} + \ldots$$

- Extract coefficients of plus (and delta) distributions from expansion coefficients around $t = 1$
- Subtract distributional part in t space and compute regular part from discontinuity as before

Generalisation: Alternative support

We discussed $x \in [0,1]$, but intermediate results can have different support

$$f(x)\theta(b-x)$$

$$\tilde{g}(N) = \int_0^b \mathrm{d}x\, x^{N-1} f(x) = b^N \int_0^1 \mathrm{d}x'\, x'^{N-1} f(bx')$$

$$\hat{f}(t) = \int_0^1 \mathrm{d}x' \frac{bt\, f(bx')}{1 - bt\, x'}$$

Generalisation: Alternative support

We discussed $x \in [0, 1]$, but intermediate results can have different support

$$f(x)\theta(b - x)$$

$$\tilde{g}(N) = \int_0^b \mathrm{d}x\, x^{N-1} f(x) = b^N \int_0^1 \mathrm{d}x'\, x'^{N-1} f(bx')$$

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{f(bx')}{\frac{x}{b} - x'}$$

Generalisation: Alternative support

We discussed $x \in [0, 1]$, but intermediate results can have different support

$$\tilde{g}(N) = \int_0^b \mathrm{d}x\, x^{N-1} f(x) = b^N \int_0^1 \mathrm{d}x'\, x'^{N-1} f(bx')$$

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{f(bx')}{\frac{x}{b} - x'}$$

$$f(x)\theta(b - x)$$

$$f(x) = \frac{-1}{2\pi \mathrm{i}} \operatorname*{Disc}_x \hat{f}\left(\frac{1}{x}\right)$$

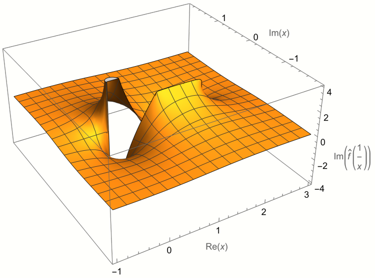
Note that the branch cut now stretches $x \in [0, b]$

Example with alternative support

$$\tilde{f}(N) = \frac{2^N}{N} \sum_{j=1}^{N-1} \frac{2^{-j}}{j}$$

$$f(x) = \begin{cases} \ln\left(\frac{2x}{2-x}\right) & 0 < x < 1 \\ \ln(2) & 1 < x < 2 \end{cases}$$

$$\hat{f}(t) = \int_0^t \frac{\mathrm{d}y}{\frac{1}{2} - y} \int_0^y \frac{\mathrm{d}z}{1 - z}$$



Connection to the optical theorem

Optical theorem:

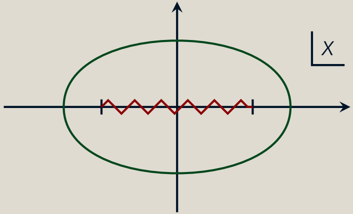
$$W^{\mu\nu} = \frac{1}{\pi} \operatorname{Im} T^{\mu\nu}$$

Hadronic tensor of DIS

Relevant variable:

$$x = \frac{Q^2}{2\,p \cdot q} \in [0, 1]$$

Analytic structure:

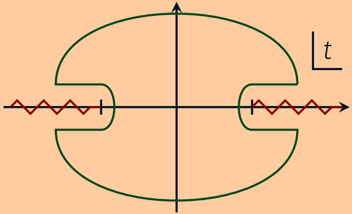


Forward Compton amplitude

Relevant variable:

$$t = \frac{2\,p \cdot q}{Q^2} \in [1, \infty[$$

Analytic structure:



Updated computational workflow

N space

- Generate diagrams & insert Feynman rules
- Simplify Dirac, Lorentz and colour algebra

t space

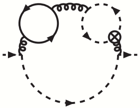
- Map integrals to integral families
- IBP reduction to master integrals (MIs)
- Derive differential equations for MIs
- Solve MIs in t space
- Assemble t space result

x space

- Translate final result from t to x space

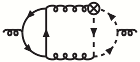
Putting the idea to use: Recent results for operator matrix elements

Previously finished three-loop operator matrix elements:



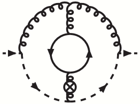
$A_{qq,Q}^{PS}$ ✓

[Ablinger et al. '10]



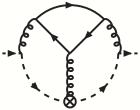
$A_{qg,Q}$ ✓

[Ablinger et al. '10]



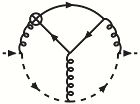
$A_{gq,Q}$ ✓

[Ablinger et al. '14a]



$A_{qq,Q}^{NS}$ ✓

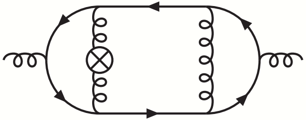
[Ablinger et al. '14b]



$A_{qq,Q}^{NS}$ ✓

[Ablinger et al. '14c]

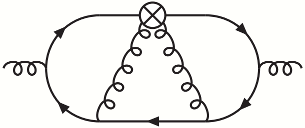
Recently finished results:



$A_{gg,Q}$ ✓

[Ablinger et al. '22]

- Complete result available
- Used t space solutions



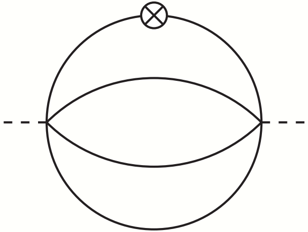
A_{Qg} (✓)

[Ablinger et al. '23]

- Partial result: All contributions from first-order factorisable differential equations
- Used t space solutions

Putting the idea to use: Finishing A_{Qg}

- Missing contributions to A_{Qg} contain MIs with non-factorisable differential equations
- All missing MIs couple to two (related) sectors with this property (see sketch on the right)



- Associated homogeneous differential equation:

$$\frac{\mathrm{d}^2 F_3(t)}{\mathrm{d}t^2} + \frac{2-t}{(1-t)t}\frac{\mathrm{d}F_3(t)}{\mathrm{d}t} + \frac{2+t}{(1-t)t(8+t)}F_3(t) = 0$$

- Homogeneous solutions

$$g_1(t) \sim \frac{{}_2F_1\left[\begin{matrix}\frac{1}{3},\frac{4}{3}\\ 2\end{matrix};-\frac{27t}{(1-t)^2(8+t)}\right]}{(1-t)^{2/3}(8+t)^{1/3}}, \qquad g_2(t) \sim \frac{{}_2F_1\left[\begin{matrix}\frac{1}{3},\frac{4}{3}\\ \frac{2}{3}\end{matrix};1+\frac{27t}{(1-t)^2(8+t)}\right]}{(1-t)^{2/3}(8+t)^{1/3}}$$

- Can be related to elliptic integrals that also appear in the three-loop ρ parameter
  [Blümlein et al. '17] [Blümlein et al. '18] [Abreu et al. '20]

Putting the idea to use: Finishing A_{Qg} (cont.)

- Full solutions can be found via variation of constants
- We find, for example, [AB, Blümlein, Schönwald '23]

$$F_3(t) = \frac{1}{\varepsilon^2}\left[\frac{10}{3} - \frac{t}{6}\right] + \frac{1}{\varepsilon}\left[-\frac{31}{6} + \frac{3t}{8} - \left(\frac{1}{3} - \frac{1}{6t} - \frac{t}{6}\right) H_1(t)\right]$$
$$+ \frac{31}{8}\ln(2) g_1(t) - \frac{31 g_2(t)}{18} + \frac{31}{18}[g_1(t)G(16;t) - g_2(t)G(10;t)]$$
$$+ \frac{1}{2}[g_2(t)G(8,1,2;t) - g_1(t)G(14,1,2;t)] + \dots$$

where the $G(\dots;t)$ are iterated integrals over the transcendental alphabet

$$\{1,\dots,17\} = \left\{\frac{1}{t}, \frac{1}{1-t}, \frac{1}{8+t}, g_1, g_2, \frac{g_1}{t}, \frac{g_1}{1-t}, \frac{g_1}{8+t}, \frac{g_1'}{t}, \frac{g_1'}{1-t}, \frac{g_1'}{8+t},\right.$$
$$\left.\frac{g_2}{t}, \frac{g_2}{1-t}, \frac{g_2}{8+t}, \frac{g_2'}{t}, \frac{g_2'}{1-t}, \frac{g_2'}{8+t}, t g_1, t g_2\right\}$$

- Solutions in t space can be translated to x space using the ideas outlined before

Conclusions

- Massive operator matrix elements are important for precision determinations of PDFs and their application to LHC phenomenology.
- All three-loop contributions related to first-order factorisable differential operators have been finished.
- We developed a method to translate t space results to x space directly.
- We calculated the first of the non-first-order factorisable master integrals in t and x space. This involves integrals over kernels depending on ${}_2F_1$ functions.
- Next goal: Calculate the remaining master integrals and complete the last missing operator matrix element A_{Qg}.

Bottom line: If you get stuck in one space look for other spaces that are more accesible!