



Towards N³LO: three-loop form factors

5th Workstop / Thinkstart: Radiative corrections and Monte Carlo tools for Strong 2020 | June 5 - 9, 2023

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Motivation





- Form factors are basic building blocks for many physical observables:
 - $t\bar{t}$ production at hadron and e^+e^- colliders
 - Higgs production and decay
 - Low-energy e^+e^- collisions and μe scattering
 - ...
- Form factors exhibit an universal infrared behavior which is interesting to study

The process





$$egin{aligned} X(q) & o Q(q_1) + ar{Q}(q_2) \ q_1^2 = q_2^2 = m^2, \quad q^2 = s = \hat{s} \cdot m^2 \end{aligned}$$

vector : axial-vector : scalar : pseudo-scala

$$\begin{aligned} J_{\mu}^{\mathsf{v}} &= \overline{\psi} \gamma_{\mu} \psi, \qquad \Gamma_{\mu}^{\mathsf{v}} &= F_{1}^{\mathsf{v}}(s) \gamma_{\mu} - \frac{\mathsf{i}}{2m} F_{2}^{\mathsf{v}}(s) \sigma_{\mu\nu} q^{\nu} \\ J_{\mu}^{\mathsf{a}} &= \overline{\psi} \gamma_{\mu} \gamma_{5} \psi, \qquad \Gamma_{\mu}^{\mathsf{a}} &= F_{1}^{\mathsf{a}}(s) \gamma_{\mu} \gamma_{5} - \frac{1}{2m} F_{2}^{\mathsf{a}}(s) q_{\mu} \gamma_{5} \\ J_{\mu}^{\mathsf{s}} &= m \overline{\psi} \psi, \qquad \Gamma^{\mathsf{s}} &= m F^{\mathsf{s}}(s) \\ \mathsf{ar}: \quad J^{\mathsf{p}} &= \mathsf{i} m \overline{\psi} \gamma_{5} \psi, \qquad \Gamma^{\mathsf{p}} &= \mathsf{i} m F^{\mathsf{p}}(s) \gamma_{5} \end{aligned}$$



Types of contributions



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Status of massive QCD corrections

nonsinglet:

00000

0000000

singlet:

m' = m



- fermionic contributions [Hoang, Teubner 1997]
- QED [Bonciani, Mastrolia, Remiddi 2003]
- complete (except contributions with $m' \neq m$) [Bernreuther, Bonciani, Gehrmann, Heinesch, Leineweber, Mastrolia, Remiddi 2004 2005]
- $F_{i}^{(3)}$ (**NNNLO**):
 - nonsinglet large N_c [Henn, Smirnov, Smirnov, Steinhauser 2016; Lee, Smirnov, Smirnov, Steinhauser 2018; Ablinger, Blümlein, Marquard, Rana, Schneider 2 × 2018; Lee, Smirnov, Smirnov, Steinhauser 2018]
 - nonsinglet n_I [Lee, Smirnov, Smirnov, Steinhauser 2018; Ablinger, Blümlein, Marquard, Rana, Schneider 2 × 2018]
 - nonsinglet n_h (partially) [Blümlein, Marquard, Rana, Schneider 2019]
 - complete (except contributions with $m' \neq m$) [Fael, FL, Schönwald, Steinhauser 2 × 2022 + 2023]



Setup



- Generate diagrams with qgraf [Nogueira 1991]
- Map to predefined integral families with q2e/exp [Harlander, Seidensticker, Steinhauser 1998; Seidensticker 1999]
- FORM [Vermaseren 2000; Kuipers, Ueda, Vermaseren, Vollinga 2013; Ruijl, Ueda, Vermaseren 2017] for Lorentz, Dirac, and color algebra [van Ritbergen, Schellekens, Vermaseren 1998]
- Reduction to master integrals with Kira [Maierhöfer, Usovitsch, Uwer 2017; Klappert, FL, Maierhöfer, Usovitsch 2020] and Fermat [Lewis]
 - Construct good basis where denominators factorize in ϵ and \hat{s} with ImproveMasters.m [Smirnov, Smirnov 2020]
- Establish differential equations in ŝ with LiteRed [Lee 2012 + 2013]

Algorithm to solve master integrals (I)



$$rac{\partial}{\partial \hat{\mathbf{s}}} M_n = A_{nm}(\epsilon, \hat{\mathbf{s}}) M_m$$

• Compute expansion around $\hat{s} = 0$ by:

Inserting an ansatz for the master integrals into the differential equation:

$$M_n(\epsilon, \hat{m{s}}=0) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{\max}} c_{ij}^{(n)} \, \epsilon^i \, \hat{m{s}}^j$$

• Compare coefficients in ϵ and \hat{s} to establish linear system of equations for $c_{ij}^{(n)}$:

$$c_{12}^{(1)}\epsilon\hat{s}^2 + \dots = 52c_{33}^{(1)}\epsilon\hat{s}^2 + \dots + 127c_{14}^{(4)}\epsilon\hat{s}^2 + \dots$$

Solve system in terms of small number of boundary constants using Kira with FireFly [Klappert, FL 2019; Klappert, Klein, FL 2020]:

$$c_{12}^{(1)} = 52c_{33}^{(1)} + 127c_{14}^{(4)}$$

Compute boundary values to fix remaining constants

Algorithm to solve master integrals (II)



$$rac{\partial}{\partial \hat{s}} M_n = A_{nm}(\epsilon, \hat{s}) M_m$$

• Repeat for $\hat{s} = \hat{s}_1$:

• Insert an ansatz around $\hat{s} = \hat{s}_1$ into the differential equation:

$$M_n(\epsilon, \hat{\mathbf{s}} = \hat{\mathbf{s}}_1) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{\text{max}}} c_{ij}^{(n)} \epsilon^i (\hat{\mathbf{s}} - \hat{\mathbf{s}}_1)^j$$

• Compare coefficients in ϵ and \hat{s} and solve system:

$$c_{12}^{(1)}\epsilon(\hat{s}-\hat{s}_{1})^{2}+\cdots = 12c_{44}^{(1)}\epsilon(\hat{s}-\hat{s}_{1})^{2}+\cdots - 23c_{04}^{(4)}\epsilon(\hat{s}-\hat{s}_{1})^{2}+\ldots \qquad \Rightarrow \qquad c_{12}^{(1)} = 12c_{44}^{(1)}-23c_{04}^{(4)}+\cdots + 23c_{04}^{(4)}\epsilon(\hat{s}-\hat{s}_{1})^{2}+\cdots + 23c_{04}^{(4)}+\cdots + 23c_{04}^{(4)}+\cdots + 23c_{$$

- Match this new expansion to previous expansion around \$\hat{s} = 0\$ numerically in between, e.g. at \$\hat{s}_1/2\$, to fix the boundary constants
- Repeat

Calculation of boundary conditions: nonsinglet





- For s = 0 the nonsinglet master integrals reduce to 3-loop on-shell propagators:
 - Well studied in the literature [Laporta, Remiddi 1996; Melnikov, van Ritbergen 1999; Lee, Smirnov 2010]
 - Some higher-order terms were missing for our calculation
 - Using the dimensional-recurrence relations from [Lee, Smirnov 2010] we calculated them with SummerTime.m [Lee, Mingulov 2015] and PSLQ [Ferguson, Bailey, Arno 1999]

Calculation of boundary conditions: singlet





- n_h singlet boundary conditions require asymptotic expansion due to massless cuts:
 - Reveal regions with ASY.m [Smirnov, Pak 2010; Jantzen, Smirnov, Smirnov 2012]
 - Naive region same as for nonsinglet
 - Remaining regions can be integrated directly or with HyperInt [Panzer 2014]

Calculation of boundary conditions: singlet





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 - Naive region same as for nonsinglet
 - Remaining regions can be integrated directly or with HyperInt [Panzer 2014]
- n_l singlet boundary conditions:
 - Even more massless cuts and direct integration for some regions too complicated
 - Instead use AMFlow [Liu, Ma 2022] to compute them numerically at $\hat{s} = -1$ with 86 digits



Example



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Example





Example



Results – analytic expansion around $\hat{s} = 0$

$$\begin{split} F_{1}^{\text{v,f,(3)}}(\hat{s}=0) &= \left\{ C_{\text{F}}^{3} \Big(-15a_{4} - \frac{17\pi^{2}\hat{\zeta}_{3}}{24} - \frac{18367\hat{\zeta}_{3}}{1728} + \frac{25\hat{\zeta}_{5}}{8} - \frac{5l_{2}^{4}}{8} - \frac{19}{40}\pi^{2}l_{2}^{2} + \frac{4957\pi^{2}l_{2}}{720} + \frac{3037\pi^{4}}{25920} \right. \\ &- \frac{24463\pi^{2}}{7776} + \frac{13135}{20736} \Big) + C_{\text{A}}C_{\text{F}}^{2} \Big(\frac{19a_{4}}{2} - \frac{\pi^{2}\hat{\zeta}_{3}}{9} + \frac{17725\hat{\zeta}_{3}}{3456} - \frac{55\hat{\zeta}_{5}}{32} + \frac{19l_{2}^{4}}{48} - \frac{97}{720}\pi^{2}l_{2}^{2} \\ &+ \frac{29\pi^{2}l_{2}}{240} - \frac{347\pi^{4}}{17280} - \frac{4829\pi^{2}}{10368} + \frac{707}{288} \Big) + C_{\text{A}}^{2}C_{\text{F}} \Big(-a_{4} + \frac{7\pi^{2}\hat{\zeta}_{3}}{96} + \frac{4045\hat{\zeta}_{3}}{5184} - \frac{5\hat{\zeta}_{5}}{64} - \frac{l_{2}^{4}}{24} \\ &+ \frac{67}{360}\pi^{2}l_{2}^{2} - \frac{5131\pi^{2}l_{2}}{2880} + \frac{67\pi^{4}}{8640} + \frac{172285\pi^{2}}{186624} - \frac{7876}{2187} \Big) \Big\} \hat{s} + \text{fermionic corrections} + \mathcal{O}(\hat{s}^{2}) \end{split}$$

•
$$I_2 = \ln(2), a_4 = \text{Li}_4(1/2) \text{ and } C_A = 3, C_F = \frac{4}{3} \text{ for QCD}$$

• Expansions for all currents are available up to $\mathcal{O}(\hat{s}^{67})$



Results – high-energy limit

$$\begin{split} F_{1}^{v,l,(3)} \Big|_{s \to -\infty} &= 4.7318 C_{\rm F}^{3} - 20.762 C_{\rm F}^{2} C_{\rm A} + 8.3501 C_{\rm F} G_{\rm A}^{2} + \left[3.4586 C_{\rm F}^{3} - 4.0082 C_{\rm F}^{2} C_{\rm A} - 6.3561 C_{\rm F} G_{\rm A}^{2} \right] l_{s} \\ &+ \left[1.4025 C_{\rm F}^{3} + 0.51078 C_{\rm F}^{2} C_{\rm A} - 2.2488 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{2} + \left[0.062184 C_{\rm F}^{3} + 0.90267 C_{\rm F}^{2} C_{\rm A} - 0.42778 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{3} \\ &+ \left[- 0.075860 C_{\rm F}^{3} + 0.20814 C_{\rm F}^{2} C_{\rm A} - 0.035011 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{4} + \left[- 0.023438 C_{\rm F}^{3} + 0.019097 C_{\rm F}^{2} C_{\rm A} \right] l_{s}^{5} \\ &+ \left[- 0.0026042 C_{\rm F}^{3} \right] l_{s}^{6} - \left\{ - 92.918 C_{\rm F}^{3} + 123.65 C_{\rm F}^{2} C_{\rm A} - 47.821 C_{\rm F} C_{\rm A}^{2} + \left[- 10.381 C_{\rm F}^{3} + 2.3223 C_{\rm F}^{2} C_{\rm A} \right] l_{s}^{4} \\ &+ 17.305 C_{\rm F} C_{\rm A}^{2} \right] l_{s} + \left[4.9856 C_{\rm F}^{3} - 19.097 C_{\rm F}^{2} C_{\rm A} + 8.0183 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{2} + \left[3.0499 C_{\rm F}^{3} - 6.8519 C_{\rm F}^{2} C_{\rm A} + 1.9149 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{4} \\ &+ \left[0.67172 C_{\rm F}^{3} - 0.91213 C_{\rm F}^{2} C_{\rm A} + 0.24069 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{4} + \left[0.13229 C_{\rm F}^{3} - 0.051389 C_{\rm F}^{2} C_{\rm A} + 0.0043403 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{5} \\ &+ \left[0.0041667 C_{\rm F}^{3} - 0.0010417 C_{\rm F}^{2} C_{\rm A} - 0.00052083 C_{\rm F} C_{\rm A}^{2} \right] l_{s}^{6} \right\} \frac{m^{2}}{s} + \mathcal{O} \left(\frac{m^{4}}{s^{2}} \right) + \text{fermionic contributions} \end{split}$$



Results – high-energy limit

$$\begin{split} F_{1}^{\text{v}1,(3)}\Big|_{s \to -\infty} &= 4.7318C_{\text{F}}^{3} - 20.762G_{\text{F}}^{2}C_{\text{A}} + 8.3501C_{\text{F}}C_{\text{A}}^{2} + \left[3.4586C_{\text{F}}^{3} - 4.0082G_{\text{F}}^{2}C_{\text{A}} - 6.3561C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{4} \\ &+ \left[1.4025C_{\text{F}}^{3} + 0.51078C_{\text{F}}^{2}C_{\text{A}} - 2.2488C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{2} + \left[0.062184C_{\text{F}}^{3} + 0.90267C_{\text{F}}^{2}C_{\text{A}} - 0.42778C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{3} \\ &+ \left[-0.075860C_{\text{F}}^{3} + 0.20814C_{\text{F}}^{2}C_{\text{A}} - 0.035011C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{4} + \left[-0.023438C_{\text{F}}^{3} + 0.019097C_{\text{F}}^{2}C_{\text{A}}\right]l_{s}^{5} \\ &+ \left[\left[-0.0026042C_{\text{F}}^{3}\right]l_{s}^{6}\right] - \left\{-92.918C_{\text{F}}^{3} + 123.65C_{\text{F}}^{2}C_{\text{A}} - 47.821C_{\text{F}}C_{\text{A}}^{2} + \left[-10.381C_{\text{F}}^{3} + 2.3223C_{\text{F}}^{2}C_{\text{A}} \right]l_{s}^{4} \\ &+ 17.305C_{\text{F}}C_{\text{A}}^{2}\right]l_{s} + \left[4.9856C_{\text{F}}^{3} - 19.097C_{\text{F}}^{2}C_{\text{A}} + 8.0183C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{2} + \left[3.0499C_{\text{F}}^{3} - 6.8519C_{\text{F}}^{2}C_{\text{A}} + 1.9149C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{5} \\ &+ \left[0.67172C_{\text{F}}^{3} - 0.91213C_{\text{F}}^{2}C_{\text{A}} + 0.24069C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{4} + \left[0.13229C_{\text{F}}^{3} - 0.051389C_{\text{F}}^{2}C_{\text{A}} + 0.0043403C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{5} \\ &+ \left[\left[0.0041667C_{\text{F}}^{3} - 0.0010417C_{\text{F}}^{2}C_{\text{A}} - 0.00052083C_{\text{F}}C_{\text{A}}^{2}\right]l_{s}^{6}\right]\right\}\frac{m^{2}}{s} + \mathcal{O}\left(\frac{m^{4}}{s^{2}}\right) + \text{fermionic contributions} \end{split}$$

Dedicated calculation of leading logarithms [Liu, Penin, Zerf 2017]:

$$F_{1}^{\rm vf,(3)} = -\frac{C_{\rm F}^{3}}{384} I_{\rm s}^{6} - \frac{m^{2}}{s} \left(\frac{C_{\rm F}^{3}}{240} - \frac{C_{\rm F}^{2}C_{\rm A}}{960} - \frac{C_{\rm F}C_{\rm A}^{2}}{1920} \right) I_{\rm s}^{6} + \dots, \quad \text{with } I_{\rm s} = \ln\left(\frac{m^{2}}{-s}\right) I_{\rm s}^{6} + \dots,$$

• We reproduce these terms with high precision



Results – pole cancellation

- We use the pole cancellation to estimate the precision
- To estimate the number of significant digits we use

$$\log_{10} \left(\left| \frac{\text{expansion} - \text{analytic CT}}{\text{analytic CT}} \right| \right)$$

- \Rightarrow We estimate at least 8 correct digits for the finite terms for QCD and 10 correct digits for QED
- Most regions for most color factors and especially singlet contributions much more precise





Results – some plots: nonsinglet





Results - some plots: singlet



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Public implementation - Mathematica



 Bare as well as both ultraviolet and infrared finite form factors implemented as grids for Mathematica: formfactors3l

```
Get["FormFactors3l.m"]
```

```
In[] := FormFactorBareNonSing[veF1, 0, -1]
Out[] := 77.0506 cA^2 cR+95.0634 cA cR^2+0.467466 cR^3
        -21.9243 cA cR I2R nh-11.5582 cR^2 I2R nh+0.751403 cR I2R^2 nh^2
        -62.6063 cA cR I2R nl-45.5408 cR^2 I2R nl+9.35837 cR I2R^2 nh nl
        +11.8102 cR I2R^2 nl^2
```

```
In[] := FormFactorRenNonSing[veF1, -1]
```

```
Out[] := 3.10714 cA^2 cR-3.23413 cA cR^2+0.0144347 cR^3
+0.0435081 cA cR I2R nh-0.0640418 cR^2 I2R nh
-0.0107609 cR I2R^2 nh^2-2.59041 cA cR I2R nl
+1.02032 cR^2 I2R nl+0.000282528 cR I2R^2 nh nl
+0.494057 cR I2R^2 nl^2
```

Public implementation – Fortran



- Ultraviolet renormalized, infrared unsubtracted form factors implemented as grids in Fortran library ff31
- Specialization to QED by adding suffix _qed to function calls
- Ready for Monte-Carlo tools

```
program example1
  use ff3l
  implicit none
  double complex :: flv
  double precision :: s = 10
  integer :: eporder
  do eporder = -3,0
    f1v = ff3l_veF1(s,eporder)
    print *,"F1( s = ",s,", ep = ",eporder," ) = ", f1v
  enddo
end program example1
```



Summary

- Calculated massive form factors at NNNLO in QCD
- Applied a semianalytic method by constructing series expansions and matching numerically
- Reproduce known results from the literature:
 - large- N_c limit, n_l , and partial n_h contributions
 - static, high-energy, and threshold expansions
- Checked chiral Ward identity for singlet contributions
- Estimate precision to at least 8 significant digits over the whole real axis for QCD and 10 significant digits for QED
- Results available as grids for both Mathematica and Fortran

Outlook: contributions with a second mass $m' \neq m$ (extremely preliminary)





NNLO:

- 1 bubble diagram
- Can be expressed through dispersion integral over vacuum polarization as for the hadronic corrections [Fael 2018]
- Leptonic vacuum polarization known through four loops in QED [Sturm 2013] and top contribution to three loops in QCD [Chetyrkin, Kühn, Steinhauser 1995 + 1996]
- NNNLO:
 - 42 nonsinglet diagrams, some of them with topologies beyond bubbles
 - 152 master integrals
 - Boundaries at s = 0 available, but already complicated functions of ratio $\frac{m'}{m}$ [Fael, Schönwald, Steinhauser 2020]
 - Then symbolic expansions in $\frac{m'}{m}$ and $\frac{s}{m}$ and match numerically?
 - Or solve numerically in relevant range $\frac{s}{m}$ for fixed $\frac{m'}{m}$ like [Boughezal, Czakon, Schutzmeier 2007; Czakon, Niggetiedt 2020] ?



Why numerical?



Large-N_c and n_l contributions at NNNLO can be written as iterated integrals over letters

$$\frac{1}{x}, \ \frac{1}{1+x}, \ \frac{1}{1-x}, \ \frac{1}{1-x+x^2}, \ \frac{x}{1-x+x^2}$$

- n_h terms already contain structures beyond iterated integrals (elliptic integrals)
- \Rightarrow No ready-to-use tools available for analytic solution
- \Rightarrow Instead: Full solution through analytic series expansions and numerical matching



Different ansätze for different points:

regular point:

$$M_n(\epsilon, \hat{s} = \hat{s}_0) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{max}} c_{ij}^{(n)} \epsilon^i (\hat{s} - \hat{s}_0)^j$$



 $s = \pm \infty$ (high-energy limit):

Different ansätze for different points:

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$$egin{aligned} &M_n(\epsilon, \hat{m{s}} = \hat{m{s}}_0) = \sum\limits_{i=-3}^\infty \sum\limits_{j=0}^{j_{ ext{max}}} c_{ij}^{(n)} \, \epsilon^i \, (\hat{m{s}} - \hat{m{s}}_0)^j \ &M_n(\epsilon, \hat{m{s}} o \pm\infty) = \sum\limits_{i=-3}^\infty \sum\limits_{j=-s_{ ext{min}}}^{j_{ ext{max}}} \sum\limits_{k=0}^{i+6} c_{ijk}^{(n)} \, \epsilon^i \, \hat{m{s}}^{-j} \, \ln^k(\hat{m{s}}) \end{aligned}$$



Different ansätze for different points:

regular point:

 $s=\pm\infty$ (high-energy limit):

 $s = 4m^2$ (2-particle threshold):

$$\begin{split} & \textit{M}_{\textit{n}}(\epsilon, \hat{s} = \hat{s}_{0}) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{max}} c_{ij}^{(n)} \, \epsilon^{i} \, (\hat{s} - \hat{s}_{0})^{j} \\ & \textit{M}_{\textit{n}}(\epsilon, \hat{s} \to \pm \infty) = \sum_{i=-3}^{\infty} \sum_{j=-s_{min}}^{j_{max}} \sum_{k=0}^{i+6} c_{ijk}^{(n)} \, \epsilon^{i} \, \hat{s}^{-j} \, \ln^{k} \left(\hat{s} \right) \\ & \textit{M}_{\textit{n}}(\epsilon, \hat{s} = 4) = \sum_{i=-3}^{\infty} \sum_{j=-s_{min}}^{j_{max}} \sum_{k=0}^{i+3} c_{ijk}^{(n)} \, \epsilon^{i} \, \left[\sqrt{4 - \hat{s}} \right]^{j} \, \ln^{k} \left(\sqrt{4 - \hat{s}} \right) \end{split}$$



Different ansätze for different points:

regular point:

 $s = \pm \infty$ (high-energy limit):

 $s = 4m^2$ (2-particle threshold):

 $M_n(\epsilon, \hat{s}
ightarrow \pm \infty) = \sum_{i=1}^{\infty} \sum_{j=1}^{j_{max}} \sum_{i=1}^{i+6} c_{ijk}^{(n)} \epsilon^i \, \hat{s}^{-j} \, \ln^k(\hat{s})$ i = -3 $i = -s_{min}$ $M_n(\epsilon, \hat{s} = 4) = \sum_{i=1}^{\infty} \sum_{j=1}^{j_{\text{max}}} \sum_{i=1}^{i+3} c_{ijk}^{(n)} \epsilon^i \left[\sqrt{4-\hat{s}}
ight]^j \ln^k \left(\sqrt{4-\hat{s}}
ight)$ $s = 16m^2 \text{ (4-particle threshold):} \quad M_n(\epsilon, \hat{s} = 16) = \sum_{i=-3}^{\infty} \sum_{j=-s}^{j_{max}} \sum_{k=0}^{i+3} c_{ijk}^{(n)} \epsilon^i \left[\sqrt{16-\hat{s}}\right]^j \ln^k \left(\sqrt{16-\hat{s}}\right)^{i-1}$

 $M_n(\epsilon, \hat{\mathbf{s}} = \hat{\mathbf{s}}_0) = \sum_{i=-3}^{\infty} \sum_{i=0}^{j_{\text{max}}} c_{ij}^{(n)} \epsilon^i (\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)^j$



Different ansätze for different points:

regular point:

 $s = 16m^2$

 $s = \pm \infty$ (

 $s = 4m^2$ (

int:

$$M_{n}(\epsilon, \hat{\mathbf{s}} = \hat{\mathbf{s}}_{0}) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{max}} c_{ij}^{(n)} \epsilon^{i} (\hat{\mathbf{s}} - \hat{\mathbf{s}}_{0})^{j}$$
(high-energy limit):

$$M_{n}(\epsilon, \hat{\mathbf{s}} \to \pm \infty) = \sum_{i=-3}^{\infty} \sum_{j=-s_{min}}^{j_{max}} \sum_{k=0}^{i+6} c_{ijk}^{(n)} \epsilon^{i} \hat{\mathbf{s}}^{-j} \ln^{k} (\hat{\mathbf{s}})$$
2-particle threshold):

$$M_{n}(\epsilon, \hat{\mathbf{s}} = 4) = \sum_{i=-3}^{\infty} \sum_{j=-s_{min}}^{j_{max}} \sum_{k=0}^{i+3} c_{ijk}^{(n)} \epsilon^{i} [\sqrt{4-\hat{\mathbf{s}}}]^{j} \ln^{k} (\sqrt{4-\hat{\mathbf{s}}})$$
(4-particle threshold):

$$M_{n}(\epsilon, \hat{\mathbf{s}} = 16) = \sum_{i=-3}^{\infty} \sum_{j=-s_{min}}^{j_{max}} \sum_{k=0}^{i+3} c_{ijk}^{(n)} \epsilon^{i} [\sqrt{16-\hat{\mathbf{s}}}]^{j} \ln^{k} (\sqrt{16-\hat{\mathbf{s}}})$$

• We construct expansions up to $j_{max} = 50$ around

$$\hat{s} = \{-\infty, -32, -28, -24, -16, -12, -8, -4, 0, 1, 2, 5/2, 3, 7/2, 4, \\ {}^{9}\!/_{2}, 5, 6, 7, 8, 10, 12, 14, 15, 16, 17, 19, 22, 28, 40\}$$

and similar for the $n_{\rm h}$ -singlet contributions



Calculation of boundary conditions – *n*_h-singlets



- The singlet diagrams can have massless cuts, therefore the limit ŝ → 0 demands an asymptotic expansion.
- We reveal regions with ASY.m [Smirnov, Pak 2010; Jantzen, Smirnov, Smirnov 2012] ($y = \sqrt{-\hat{s}}$):
 - $\checkmark y^{-0\epsilon}$: taylor expansion of the integrand, same as for the non-singlet
 - ✓ $y^{-2\epsilon}$: integrals can be performed for general ϵ in terms of Γ functions
 - \checkmark y^{-4 ϵ}: one integral was calculated using HyperInt [Panzer 2014]
- \Rightarrow We obtain analytic boundary conditions in the limit $\hat{s} \rightarrow 0$.

Calculation of boundary conditions – *n*_l-singlets



- The singlet diagrams can have massless cuts, therefore the limit ŝ → 0 demands an asymptotic expansion.
- We reveal regions with ASY.m [Smirnov, Pak 2010; Jantzen, Smirnov, Smirnov 2012] ($y = \sqrt{-\hat{s}}$):
 - $\checkmark y^{-0\epsilon}$: taylor expansion of the integrand, same as for the non-singlet
 - ✓ $y^{-2\epsilon}$: integrals can be performed for general ϵ in terms of Γ functions
 - $\checkmark y^{-4\epsilon}$: integrals can be performed with HyperInt and Mellin-Barnes methods
 - × $y^{-6\epsilon}$: direct integration for some integrals quite involved
- \Rightarrow For the n_l -singlets we changed strategy and calculated the masters at $\hat{s} = -1$ with AMFLow [Liu, Ma 2022] and matched from there.

Karlsruhe Institute of Technology

Moebius Transformations

- The radius of convergence is at most the distance to the closest singularity.
- We can extend the radius of convergence by changing to a new expansion variable.
- If we want to expand around the point x_k with the closest singularities at x_{k-1} and x_{k+1} , we can use:

$$y_k = rac{(x-x_k)(x_{k+1}-x_{k-1})}{(x-x_{k+1})(x_{k-1}-x_k)+(x-x_{k-1})(x_{k+1}-x_k)}$$

• The variable change maps $\{x_{k-1}, x_k, x_{k+1}\} \rightarrow \{-1, 0, 1\}$.

Renormalization and infrared structure



UV renormalization

- $\overline{\mathrm{MS}}$ renormalization of α_{s}
- On-shell renormalization of mass Z^{OS}_m, wave function Z^{OS}₂, and (if needed) currents [Chetyrkin, Steinhauser 1999; Melnikov, van Ritbergen 2000]
- Much more involved renormalization for the axial and pseudoscalar singlet contributions

IR subtraction

- Structure of infrared poles given by cusp anomalous dimension Γ_{cusp} [Grozin, Henn, Korchemski, Marquard 2014]
- Define finite form factors $F = Z_{IR}F^{finite}$ with UV-renormalized form factor F and

$$Z_{\text{IR}} = 1 - \frac{\alpha_s}{\pi} \frac{1}{2\epsilon} \Gamma_{\text{cusp}}^{(1)} - \left(\frac{\alpha_s}{\pi}\right)^2 \left(\frac{\cdots}{\epsilon^2} + \frac{1}{4\epsilon} \Gamma_{\text{cusp}}^{(2)}\right) - \left(\frac{\alpha_s}{\pi}\right)^3 \left(\frac{\cdots}{\epsilon^3} + \frac{\cdots}{\epsilon^2} + \frac{1}{6\epsilon} \Gamma_{\text{cusp}}^{(3)}\right)$$

- $\Gamma_{\text{cusp}} = \Gamma_{\text{cusp}}(x)$ depends on kinematics
- Γ_{cusp} universal for all currents

Treatment of γ_5

- For non-singlet diagrams always an even number of γ_5 matrices appear on a fermion line.
 - \Rightarrow Use anti-commuting γ_5 .
- $\hfill \hfill \hfill$
 - \Rightarrow Use Larin's prescription [Larin 1992] :

- where the contraction of two ϵ tensors is done in $d = 4 2\epsilon$ dimensions.
- ✓ Finite (multiplicative) renormalization constants for all currents are known.
- Only the sum of singlet and non-singlet diagrams renormalizes multiplicative, so the non-singlet has to be calculated in the Larin scheme as well (we use this as a cross-check).



$$\gamma_{\mu}\gamma_{5}
ightarrow rac{1}{3!} \epsilon_{\mu
u
ho\sigma}\gamma^{
u}\gamma^{
ho}\gamma^{\sigma} ,$$



Chiral Ward identity



The non-renormalization of the Adler-Bell-Jackiw (ABJ) anomaly implies:

$$\left(\partial^{\mu}j^{a}_{\mu}\right)_{\mathsf{R}}=2\left(j^{p}\right)_{\mathsf{R}}+\frac{\alpha_{s}}{4\pi}\mathcal{T}_{\mathsf{F}}\left(\tilde{G}\tilde{G}\right)_{\mathsf{R}}$$

- with the pseudoscalar gluonic operator $G ilde{G} = \epsilon_{\mu
 u
 ho \sigma} G^{a,\mu
 u} G^{a,
 ho \sigma}$
- This relation can be used to check the correct treatment of γ₅.
- For the form factors this leads to the identity:

$$F_{\text{sing},1}^{a,f} + \frac{s}{4m^2}F_{\text{sing},2}^{a,f} = F_{\text{sing}}^{p,f} + \frac{\alpha_s}{4\pi}T_FF_{G\tilde{G}}^f$$

• We calculated the form factor associated to $G\tilde{G}$ up to $\mathcal{O}(\alpha_s^2)$ for this check.

Institute for Theoretical Particle Physics and Institute for Astroparticle Physics



Chiral Ward identity



- The new topologies introduce 3 (1), 24 (15) master integrals (new wrt. the form factor calculation).
- We calculate the masters by the algorithm outlined in [Ablinger, Blümlein, Marquard, Rana, Schneider 2018] :
 - Uncouple coupled blocks of the differential equation into a higher order one with OreSys [Gerhold 2002] and Sigma [Schneider 2007].
 - Solve the higher order differential equations via the factorization of the differential operator with HarmonicSums [Ablinger 2011-].
 - Intersection of the provide the provided the provided
- We can express the result up to $\mathcal{O}(\alpha_s^2)$ in terms of harmonic polylogarithms.

[Remiddi, Vermseren 1999]

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Results – threshold expansion around $s = 4m^2$



Close to threshold we can construct cross-sections and decay rates like

$$\sigma(e^+e^- \to Q\bar{Q}) = \sigma_0\beta \underbrace{\left(\left| F_1^{\nu} + F_2^{\nu} \right|^2 + \frac{\left| (1 - \beta^2) F_1^{\nu} + F_2^{\nu} \right|^2}{2(1 - \beta^2)} \right)}_{=3/2\,\Delta^{\nu}}$$

with the quark velocity $\beta = \sqrt{1 - 4m^2/s}$

- Real radiation suppressed by β^3
- ⇒ Direct phenomenological relevance
- We find (with $I_{2\beta} = \ln(2\beta)$)

$$\begin{split} \Delta^{\nu,(3)} &= C_{\mathsf{F}}^3 \Big[-\frac{32.470}{\beta^2} + \frac{1}{\beta} \big(14.998 - 32.470 \mathit{l}_{2\beta} \big) \Big] + C_{\mathsf{A}}^2 C_{\mathsf{F}} \frac{1}{\beta} \Big[16.586 \mathit{l}_{2\beta}^2 - 22.572 \mathit{l}_{2\beta} + 42.936 \Big] \\ &+ C_{\mathsf{A}} C_{\mathsf{F}}^2 \Big[\frac{1}{\beta^2} \big(-29.764 \mathit{l}_{2\beta} - 7.7703 \big) + \frac{1}{\beta} \big(-12.516 \mathit{l}_{2\beta} - 11.435 \big) \Big] \\ &+ \mathcal{O}(\beta^0) + \text{fermionic contributions} \end{split}$$

Agrees with dedicated calculation [Kiyo, Maier, Maierhöfer, Marquard 2009]