Singlet and anomaly contributions to massive QCD form factors

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University of Zürich

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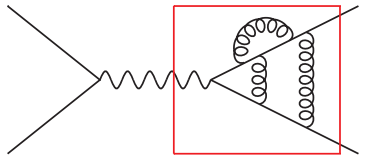
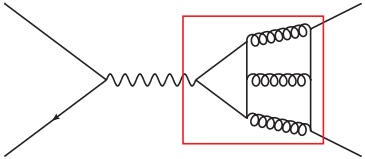
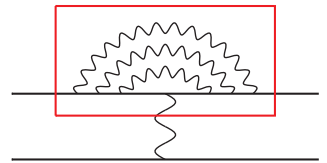
Motivation

Motivation



- Form factors are basic building blocks for many physical observables:
  - $t\,\bar{t}$ production at hadron and $e^+\,e^-$ colliders
  - $\mu\,e$ scattering
  - Higgs production and decay
  - ...
- Form factors exhibit an universal infrared behavior.



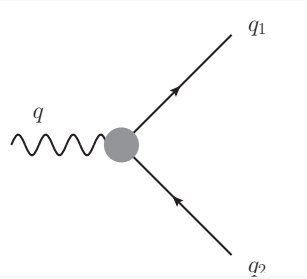


Definition and Previous Calculations

The Process

$$X(q) \to Q(q_1) + Q(q_2)$$

$$q_1^2 = q_2^2 = m^2, \qquad q^2 = s = \hat{s} \cdot m^2$$



vector : $j^v_\mu = \overline{\psi}\gamma_\mu\psi \qquad \Gamma^v_\mu = F^v_1(s)\gamma_\mu - \frac{i}{2m}F^v_2(s)\sigma_{\mu\nu}q^\nu$

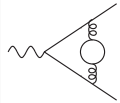
axial-vector : $j^a_\mu = \overline{\psi}\gamma_\mu\gamma_5\psi \qquad \Gamma^a_\mu = F^a_1(s)\gamma_\mu\gamma_5 - \frac{1}{2m}F^a_2(s)q_\mu\gamma_5$

scalar : $j^s = m\overline{\psi}\psi \qquad \Gamma^s = mF^s(s)$

pseudo-scalar : $j^p = im\overline{\psi}\gamma_5\psi \qquad \Gamma^p = imF^p(s)\gamma_5$

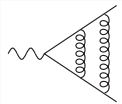
Previous Calculations

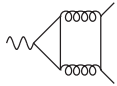
NNLO



$F_l^{(2)}$ fermionic corrections [Hoang, Teubner '97]

$F_l^{(2)}$ [Bernreuther, Bonciani, Gehrmann, Heinesch, Leineweber, Mastrolia, Remiddi '04-'06]

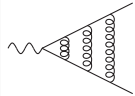




$+\mathcal{O}(\epsilon)$ [Gluza, Mitov, Moch, Riemann '09]

$+\mathcal{O}(\epsilon^2)$ [Ahmed, Henn, Steinhauser '17; Ablinger, Behring, Blümlein, Falcioni, Freitas, Marquard, Rana, Schneider '17]

NNNLO – non-singlet

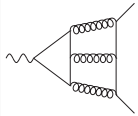


$F_l^{(3)}$ large-N_c [Henn, Smirnov, Smirnov, Steinhauser '16-'18; Ablinger, Marquard, Rana, Schneider '18]

n_l [Lee, Smirnov, Smirnov, Steinhauser '18]

n_h (partially) [Blümlein, Marquard, Rana, Schneider '19] [see also the talk of Peter Marquard]

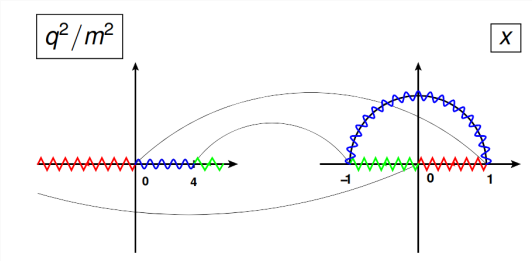
full (semi-analytic) [Fael, Lange, Schönwald, Steihauser '22]



this talk: full (semi-analytic) results for singlet diagrams at NNNLO

Previous Calculations

$$q^2 = s = -\frac{(1-x)^2}{x}$$



- The large-N_c and n_l contributions at NNNLO can be written as iterated integrals over the letters:

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

- The n_h terms already contain structures which go beyond iterated integrals.

$\Rightarrow$ We aim at the full solution through analytic series expansions and numerical matching.

Technical Details

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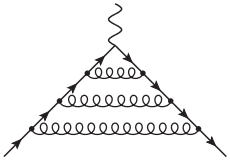
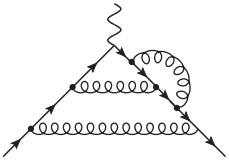
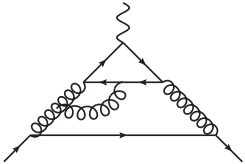

- Generate diagrams with `QGRAF`. [Nogueira '93]
- Use `FORM` [Ruijl, Ueda, Vermaseren '17] for Lorentz, Dirac and color algebra. [Ritbergen, Schellekens, Vermaseren '98]
- Map the output to predefined integral families with q2e/exp. [Harlander, Seidensticker, Steinhauser '97-'99]
- Reduce the scalar integrals to masters with `Kira`. [Klappert, Lange, Maierhöfer, Usovitsch, Uwer '17,'20]
  - We ensure a good basis where denominators factorize in ϵ and $\hat{s}$ with `ImproveMasters.m`. [Smirnov, Smirnov '20]
- Establish differential equations in variable $\hat{s}$ using `LiteRed`. [Lee '12,'14]

	non-singlet	nh-singlet	nl-singlet
diagrams	271	66	66
families	34	17	13
masters	422	316	158

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

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[Klappert, Klein, Lange '19,'20]

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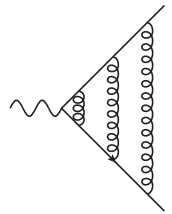
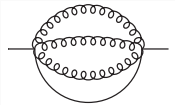
- Repeat the procedure for the next point.

Calculation of Boundary Conditions – Non-Singlet



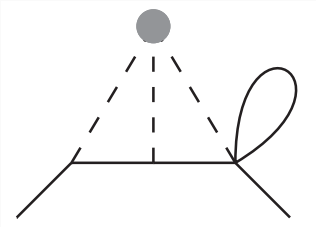
$s \to 0$

$\Longrightarrow$



- For $s = 0$ the master integrals reduce to 3-loop on-shell propagators:
  - These integrals are well studied in the literature. [Laporta, Remiddi '96; Melnikov, Ritbergen '00; Lee, Smirnov '10]
- The reduction introduces high inverse powers in ϵ, which require some integrals up to weight 9.
- We calculate the needed terms with `SummerTime.m` [Lee, Mingulov '15] and `PSLQ` [Ferguson, Bailey '92] .

Calculation of Boundary Conditions – n_h-Singlets



- The singlet diagrams can have massless cuts, therefore the limit $\hat{s} \to 0$ demands an asymptotic expansion.
- We reveal regions with `ASY.m` [Smirnov, Pak '10; Jantzen, Smirnov, Smirnov '12] $(y = \sqrt{-\hat{s}})$:
  - ✓ $y^{-0\epsilon}$: 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
  - ✓ $y^{-4\epsilon}$: one integral was calculated using `HyperInt` [Panzer '14]

$\Rightarrow$ We obtain analytic boundary conditions in the limit $\hat{s} \to 0$.

Calculation of Boundary Conditions – n_l-Singlets

- The singlet diagrams can have massless cuts, therefore the limit $\hat{s} \to 0$ demands an asymptotic expansion.
- We reveal regions with `ASY.m` [Smirnov, Pak '10; Smirnov^2, Jantzen '12] $\left(y = \sqrt{-\hat{s}}\right)$:
  - ✓ $y^{-0\epsilon}$: 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
  - ✓ $y^{-4\epsilon}$: 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 '22] and matched from there.

Series Expansions

- Special points:

$s = 0$	$s = 4m^2$	$s = 16m^2$	$s = \pm\infty$
$x = 1$	$x = -1$	$x = 4\sqrt{3} - 7$	$x = 0$
static limit	2-particle threshold	4-particle threshold	high energy limit

- Every expansion point needs a different ansatz.

$$\boxed{M_n(\epsilon, \hat{s} = 0) = \sum_{i=-3}^{\infty} \sum_{j=-j_{\min}}^{j_{\max}} \sum_{k=0}^{i+3} c_{ij}^{(n)}\, \epsilon^i \sqrt{-\hat{s}}^{\,j} \ln^k \left(\sqrt{-\hat{s}}\right)}$$

For non-singlet diagrams a simple taylor expansion in $\hat{s}$ is sufficient.

Series Expansions

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- Every expansion point needs a different ansatz.

$$M_n(\epsilon, \hat{s} = 4) = \sum_{i=-3}^{\infty} \sum_{j=-j_{\min}}^{j_{\max}} \sum_{k=0}^{i+3} c_{ijk}^{(n)} \, \epsilon^i \left[\sqrt{4 - \hat{s}}\right]^j \ln^k \left(\sqrt{4 - \hat{s}}\right)$$

Series Expansions

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$s = 0$	$s = 4m^2$	$s = 16m^2$	$s = \pm\infty$
$x = 1$	$x = -1$	$x = 4\sqrt{3} - 7$	$x = 0$
static limit	2-particle threshold	4-particle threshold	high energy limit

- Every expansion point needs a different ansatz. (only needed for the n_h singlets)

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

Series Expansions

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static limit	2-particle threshold	4-particle threshold	high energy limit

- Every expansion point needs a different ansatz.

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

Series Expansions

- Special points:

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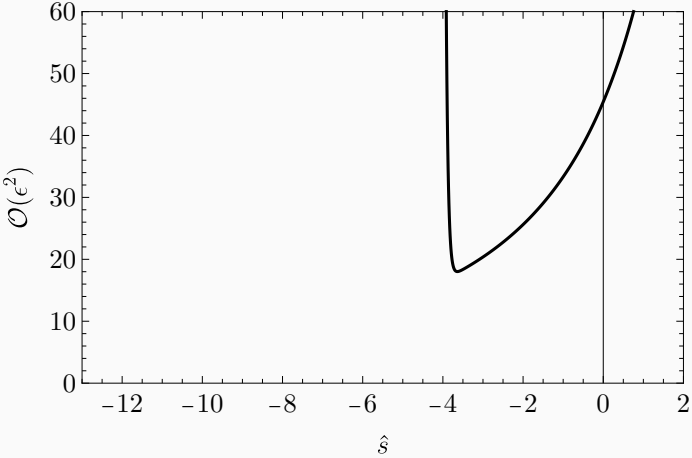
static limit	2-particle threshold	4-particle threshold	high energy limit

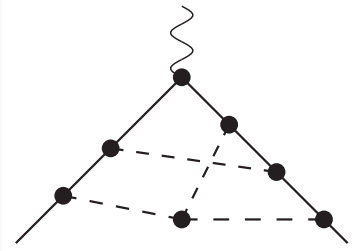
- Every expansion point needs a different ansatz.

- We construct expansions with $j_{\text{max}} = 50$ around:

$$\hat{s} = \{-\infty, -32, -28, -24, -16, -12, -8, -4, -3, -2, -1, 0, 1, 2, 3, 7/2, 4, 9/2, 5, 6, 7, 8, 10, 12, 14, 15, 16, 17, 19, 22, 28, 40, 52\}$$

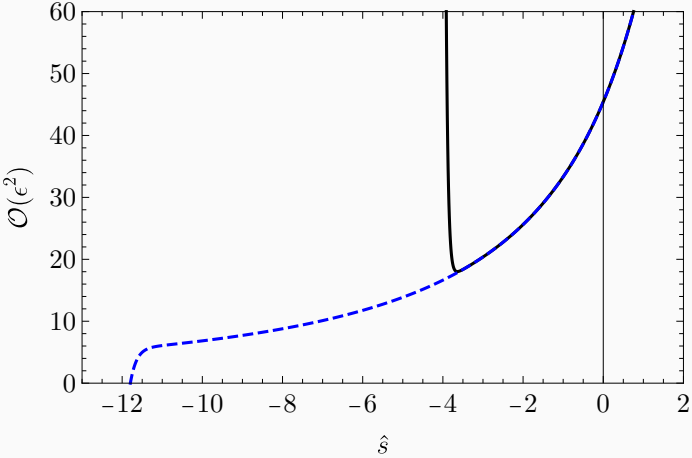
Example

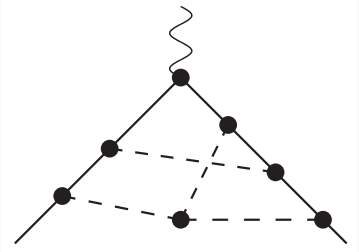




- Expansion around $\hat{s} = 0$.

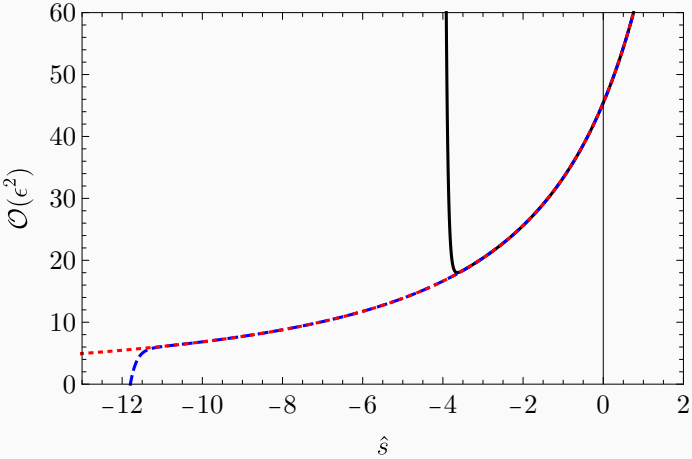
Example

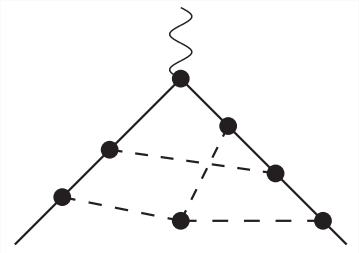




- Expansion around $\hat{s} = 0$.
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$.

Example





- Expansion around $\hat{s} = 0$.
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$.
- Expansion around $\hat{s} = -8$, matched at $\hat{s} = -6$.

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.
- In the singlet diagrams odd numbers of γ_5 appear on a fermion line.
  $\Rightarrow$ Use Larin's prescription [Larin '92] :

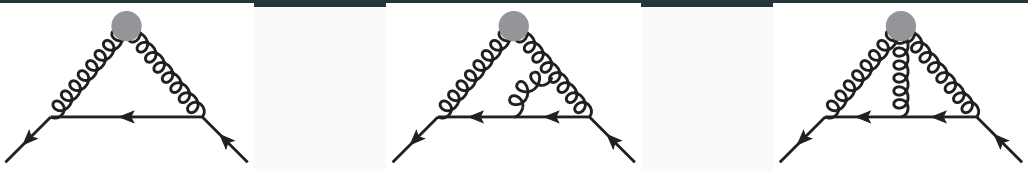
$$\boxed{\gamma_\mu \gamma_5 \to \frac{1}{3!} \epsilon_{\mu\nu\rho\sigma} \gamma^\nu \gamma^\rho \gamma^\sigma},$$

  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).

Chiral Ward Identity



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

$$\boxed{\left(\partial^\mu j^a_\mu\right)_{\mathrm{R}} = 2\left(j^p\right)_{\mathrm{R}} + \frac{\alpha_s}{4\pi} T_F \left(G\tilde{G}\right)_{\mathrm{R}}},$$

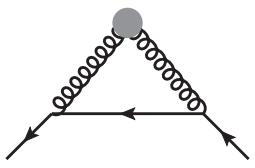
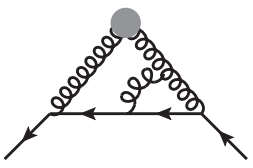
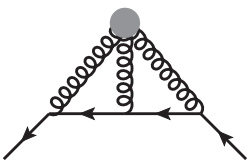
  with the pseudoscalar gluonic operator $G\tilde{G} = \epsilon_{\mu\nu\rho\sigma} G^{a,\mu\nu} G^{a,\rho\sigma}$

- This relation can be used to check the correct treatment of γ_5.
- For the form factors this leads to the identity:

$$\boxed{F^{a,f}_{\mathrm{sing},1} + \frac{s}{4m^2} F^{a,f}_{\mathrm{sing},2} = F^{p,f}_{\mathrm{sing}} + \frac{\alpha_s}{4\pi} T_F F^f_{G\tilde{G}}}$$

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

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 '18] :
  1. Uncouple coupled blocks of the differential equation into a higher order one with `OreSys` [Gerhold '02] and `Sigma` [Schneider '07] .
  2. Solve the higher order differential equations via the factorization of the differential operator with `HarmonicSums` [Ablinger '11-] .
  3. The boundary conditions can be found by direct integration in the asymptotic limit $\hat{s} \to 0$.
- We can express the result up to $\mathcal{O}(\alpha_s^2)$ in terms of harmonic polylogarithms. [Remiddi, Vermseren '99]

Results

Results – Analytic $\hat{s} = 0$ Expansion

Analytic expansion of the n_h-singlet
for $\hat{s} = 0$:

$$
\begin{aligned}
F^{s,f,(3)}_{\text{sing}}(\hat{s}=0) = T_F n_h \Bigg\{ & C_F^2 \Big(-\frac{32 a_4}{3} + \frac{55\zeta_3}{72} + \frac{445}{108} + \frac{517\pi^2}{324} - \frac{11\pi^4}{270} - \frac{4 l_2^4}{9} + \frac{4}{9}\pi^2 l_2^2 - \frac{22}{9}\pi^2 l_2 \Big) \\
& + C_A C_F \Big(\frac{22 a_4}{3} + \frac{113\zeta_3}{36} - \frac{\pi^2\zeta_3}{4} + \frac{5\zeta_5}{4} - \frac{643}{54} + \frac{466\pi^2}{81} + \frac{187\pi^4}{4320} + \frac{11 l_2^4}{36} - \frac{11}{36}\pi^2 l_2^2 - \frac{61}{9}\pi^2 l_2 \Big) \\
& + C_F T_F n_h \Big(-\frac{8\zeta_3}{3} + \frac{16}{9} + \frac{26\pi^2}{135} \Big) + C_F T_F n_l \Big(\frac{20}{9} - \frac{10\pi^2}{27} \Big) \\
& + \sqrt{-\hat{s}}\, \pi^2 \Bigg[\frac{C_F^2}{16} + C_A C_F \Big(\frac{11}{36} l_{\sqrt{-\hat{s}}} + \frac{\pi^2}{72} - \frac{263}{432} \Big) + C_F T_F n_l \Big(\frac{4}{27} - \frac{1}{9} l_{\sqrt{-\hat{s}}} \Big) \Bigg] \Bigg\} + \mathcal{O}(\hat{s})
\end{aligned}
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with $l_2 = \ln(2)$, $a_4 = \mathrm{Li}_4(1/2)$ and $C_A = 3$, $C_F = 4/3$ for QCD.

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- We have calculated the expansion up to $\mathcal{O}(s^{66})$.

Results – Pole Cancellation

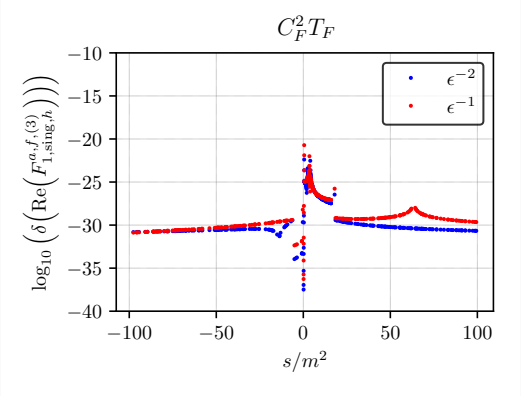
- We can use the pole cancellation to estimate the precision.

⇒ We find at least 10 significant digits, although some regions are much more precise.

- To estimate the number of significant digits we use:

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

- The analytic expressions for the poles are expressed by Harmonic Polylogarithms which can be evaluated with `ginac`. [Vollinga, Weinzierl '05]



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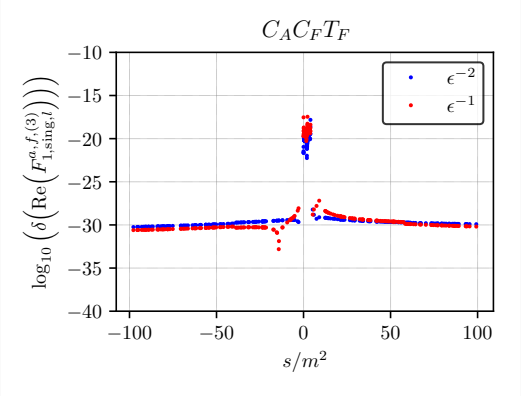

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⇒ The chiral Ward identity is fulfilled to at least the same accuracy.

- To estimate the number of significant digits we use:

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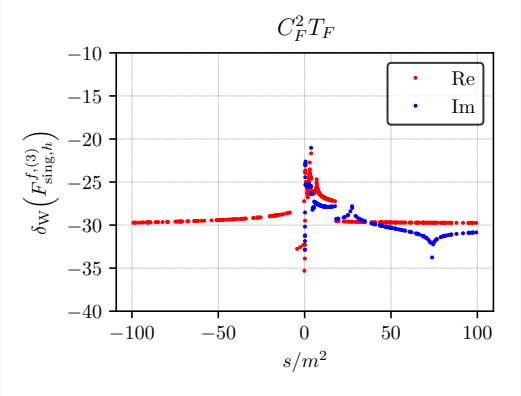
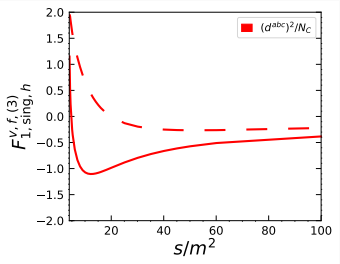
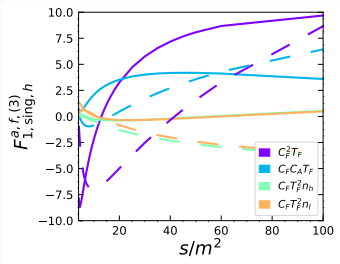
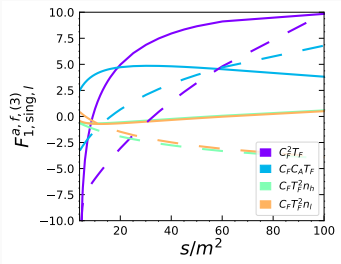
- The analytic expressions for the poles and counter terms are expressed by Harmonic Polylogarithms which can be evaluated with `ginac`. [Vollinga, Weinzierl '05]



Result – Finite Form Factors







Results – High Energy Limit

- For $s \to \infty$ there is the prediction: [Liu, Penin, Zerf '18]

$$F_{\text{sing}}^{s,f,(3)} = F_{\text{sing}}^{p,f,(3)} = -\frac{m^2}{s} l_s^6 \left(\frac{C_A C_F T_F}{960} + \frac{C_F^2 T_F}{240} \right) + \ldots, \quad \text{with } l_s = \ln\left(\frac{m^2}{-s}\right)$$

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- We obtain:

$$\begin{aligned}
F^{s,f}_{\text{sing},h}\Big|_{s\to-\infty} &= \left(\frac{\alpha_s}{\pi}\right)^2 C_F T_F \left[-\frac{1}{48} l_s^4 + \left(1 - \frac{\pi^2}{12}\right) l_s^2 + \left(4 - 3\zeta_3\right) l_s + \frac{2\pi^2}{3} - \frac{\pi^4}{45} \right] \\
&- \left(\frac{\alpha_s}{\pi}\right)^3 C_F T_F \frac{m^2}{s} \Bigg[C_F \Bigg(\boxed{0.0041667 l_s^6} - 0.0062500 l_s^5 + 0.062124 l_s^4 + 1.0817 l_s^3 + 4.8496 l_s^2 \\
&+ 32.500 l_s + 58.066 \Bigg) + C_A \Bigg(\boxed{0.0010417 l_s^6} - 0.022917 l_s^5 - 0.14492 l_s^4 + 0.46401 l_s^3 \\
&+ 3.6270 l_s^2 + 9.0468 l_s + 16.307 \Bigg) + T_F n_h \Bigg(0.0083333 l_s^5 + 0.023148 l_s^4 - 0.078904 l_s^3 \\
&- 0.31219 l_s^2 - 2.1741 l_s - 1.2446 \Bigg) + T_F n_l \Bigg(0.0083333 l_s^5 + 0.023148 l_s^4 - 0.078904 l_s^3 \\
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\end{aligned}$$

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- We obtain:

$$\begin{aligned} F^{a,f}_{2,\text{sing},l}\Big|_{s\to-\infty} &= \left(\frac{\alpha_s}{\pi}\right)^2 C_F T_F \frac{m^2}{-s}\left[-\frac{1}{2} l_s^2 - 3 l_s - 2 - \frac{\pi^2}{3}\right] \\ &+ \left(\frac{\alpha_s}{\pi}\right)^3 C_F T_F \frac{m^2}{-s}\Bigg[C_F\left(0.104167 l_s^4 + 1. l_s^3 + 6.68117 l_s^2 + 22.4839 l_s + 34.67\right) \\ &+ C_A\left(0.0208333 l_s^4 - 0.611111 l_s^3 - 7.80858 l_s^2 - 30.0535 l_s - 49.2293\right) \\ &+ T_F n_h\left(0.222222 l_s^3 + 2.05556 l_s^2 + 6.33333 l_s + 8.54753\right) \\ &+ T_F n_l\left(0.222222 l_s^3 + 2.05556 l_s^2 + 6.33333 l_s + 10.147\right)\Bigg] \end{aligned}$$

Public Implementation

- There are two public implementations for the numerical evaluation:
  1. `formfactors3l`: `Mathematica` implementation of bare and finite form factors
  2. `ff3l`: `Fortran` for ultraviolet renormalized (but infrared unsubtracted) form factors

```
program example1
  use ff3l
  implicit none

  double complex :: f1v
  double precision :: s = 10
  integer :: eporder

  call ff3l_nhsinglet_off
  do eporder = -3,0
f1v = ff3l_veF1(s,eporder)
print *,"F1( s = ",s,", ep = ",eporder," ) = ", f1v
  enddo
end program example1
```

Conclusions and Outlook

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- We have calculated the singlet contributions to the massive quark form factors at NNNLO.
- We applied a semianalytic method by constructing series expansions and numerical matching.
- We can reproduce known results in the literature.
- We estimate the precision to 10 significant digits over the whole real axis.
- We provide public Implementations for the evaluation of the massive quark form factors.
- Together with our previous non-singlet calculation the massive quark form factors are fully available at NNNLO.

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Outlook

- Calculate the contributions including a second heavy quark.

$\Rightarrow$ Interesting for muon electron scattering.

Backup

Algorithm to Solve Master Integrals

There are other approaches based on expansions:

- `SolveCoupledSystems.m` [Blümlein, Schneider '17]
- `DESS.m` [Lee, Smirnov, Smirnov '18]
- `DiffExp.m` [Hidding '20]
- `SeaSyde.m` [Armadillo, Bonciani, Devoto, Rana, Vicini '22]
- ...

Our approach ...

- ... does not require a special form of differential equation.
- ... provides approximation in whole kinematic range.
- ... is applied to physical quantity. [Fael, Lange, KS, Steinhauser '21]

Renormalization and Infrared Structure

UV renormalization

- On-shell renormalization of mass Z_m^{OS}, wave function Z_2^{OS}, and (if needed) the currents.
  [Chetyrkin, Steinhauser '99; Melnikov, Ritbergen '00]

IR subtraction

- Structure of the infrared poles is given by the cusp anomalous dimension Γ_{cusp}.
  [Grozin, Henn, Korchemski, Marquard '14]
- Define finite form factors $F = Z_{\text{IR}} F^{\text{finite}}$ with the UV renormalized form factor F and

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

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

Moebius Transformations

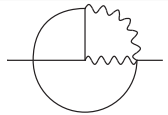
- The radius of convergence is at most the distance to the closest singularity.
- We can extend the radius of convergence by changing to a new expansion variable.
- If we want to expand around the point x_k with the closest singularities at x_{k-1} and x_{k+1}, we can use:

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

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

Calculation of Boundary Conditions

E.g. extension of G_{66} (given up to and including $\mathcal{O}(\epsilon^3)$ in [Lee, Smirnov '10]):



$$= \cdots + \epsilon^4 \Bigg(-4704 s_6 - 9120 s_{7a} - 9120 s_{7b} - 547 s_{8a} + 9120 s_6 \ln(2) + 28 \ln^4(2) + \frac{112 \ln^5(2)}{3} - \frac{808}{45} \ln^6(2)$$

$$- \frac{347}{9} \ln^8(2) + 672 \mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{5552}{3} \ln^4(2) \mathrm{Li}_4\left(\frac{1}{2}\right) - 22208 \mathrm{Li}_4\left(\frac{1}{2}\right)^2 - 4480 \mathrm{Li}_5\left(\frac{1}{2}\right) - 12928 \mathrm{Li}_6\left(\frac{1}{2}\right) + \ldots \Bigg)$$

$$+ \epsilon^5 \Bigg(14400 s_6 - \frac{377568 s_{7a}}{7} - \frac{93984 s_{7b}}{7} - 2735 s_{8a} + 7572912 s_{9a} - 3804464 s_{9b} - \frac{5092568 s_{9c}}{3} - 136256 s_{9d}$$

$$+ 681280 s_{9e} + 272512 s_{9f} + \frac{377568}{7} s_6 \ln(2) - \frac{32465121}{20} s_{8a} \ln(2) - 10185136 s_{8b} \ln(2) + 136256 s_{7b} \ln^2(2) + \ldots \Bigg)$$

$$+ \mathcal{O}(\epsilon^6)$$

Results – Threshold Expansion

- Close to threshold it is interesting to consider:

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

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

- Real radiation is supressed by β^3.
- We find (with $l_{2\beta} = \ln(2\beta)$):

$$\begin{aligned}\Delta^{(3)} = {} & C_F^3 \left[-\frac{32.470}{\beta^2} + \frac{1}{\beta}\left(14.998 - 32.470 l_{2\beta}\right) \right] + C_A^2 C_F \frac{1}{\beta}\left[16.586 l_{2\beta}^2 - 22.572 l_{2\beta} + 42.936\right] \\ & + C_A C_F^2 \left[\frac{1}{\beta^2}\left(-29.764 l_{2\beta} - 7.770339\right) + \frac{1}{\beta}\left(-12.516 l_{2\beta} - 11.435\right) \right] \\ & + \mathcal{O}(\beta^0) + \text{fermionic contributions}\end{aligned}$$