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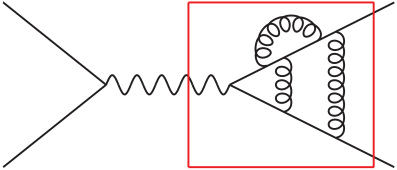
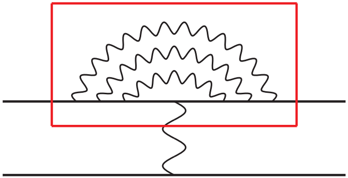
Massive quark form factors at three loops

8th International Workshop on High Precision for Hard Processes | September 20 – 22, 2022

Fabian Lange
in collaboration with Matteo Fael, Kay Schönwald, Matthias Steinhauser | Sep 20, 2022

Motivation





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

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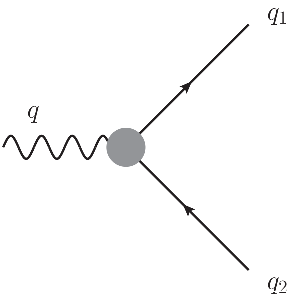
The process

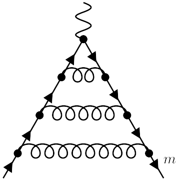


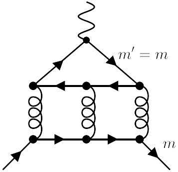
$$X(q) \to Q(q_1) + \bar{Q}(q_2)$$

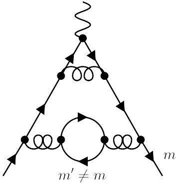
$$q_1^2 = q_2^2 = m^2, \quad q^2 = s = \hat{s} \cdot m^2$$

vector :	$j_\mu^{\mathrm{v}} = \overline{\psi}\gamma_\mu\psi,$	$\Gamma_\mu^{\mathrm{v}} = F_1^{\mathrm{v}}(s)\gamma_\mu - \frac{\mathrm{i}}{2m}F_2^{\mathrm{v}}(s)\sigma_{\mu\nu}q^\nu$
axial-vector :	$j_\mu^{\mathrm{a}} = \overline{\psi}\gamma_\mu\gamma_5\psi,$	$\Gamma_\mu^{\mathrm{a}} = F_1^{\mathrm{a}}(s)\gamma_\mu\gamma_5 - \frac{1}{2m}F_2^{\mathrm{a}}(s)q_\mu\gamma_5$
scalar :	$j^{\mathrm{s}} = m\overline{\psi}\psi,$	$\Gamma^{\mathrm{s}} = mF^{s}(s)$
pseudo-scalar :	$j^{\mathrm{p}} = \mathrm{i}m\overline{\psi}\gamma_5\psi,$	$\Gamma^{\mathrm{p}} = \mathrm{i}mF^{\mathrm{p}}(s)\gamma_5$

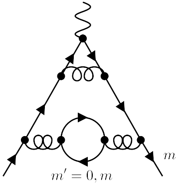
Types of contributions

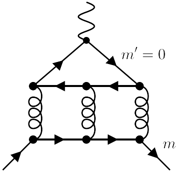


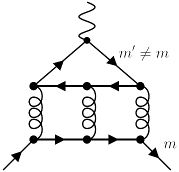




n_h singlet







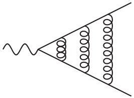
nonsinglet

n_l singlet

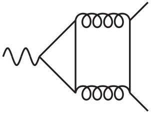
contributions with $m' \neq m$

Status of massive QCD corrections

nonsinglet:



singlet:



$F_i^{(2)}$ (**NNLO**):

- fermionic contributions [Hoang, Teubner 1997]
- complete [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 $\times$ 2018; Lee, Smirnov, Smirnov, Steinhauser 2018]
- nonsinglet n_l [Lee, Smirnov, Smirnov, Steinhauser 2018; Ablinger, Blümlein, Marquard, Rana, Schneider 2 $\times$ 2018]
- nonsinglet n_h (partially) [Blümlein, Marquard, Rana, Schneider 2019]

This talk: full (numerical) results for nonsinglet and n_h-singlet contributions at NNNLO

Status of massive QCD corrections

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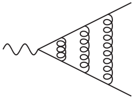

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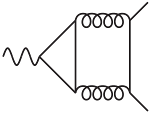

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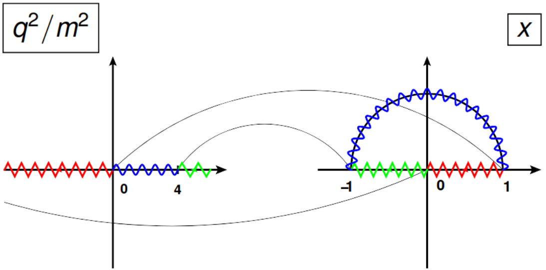
Status for massless form factors:

- $F_i^{(4)}$ computed recently [Lee, von Manteuffel, Schabinger, Smirnov, Smirnov, Steinhauser 2022] $\Rightarrow$ Matthias Steinhauser's talk
- Singlet contributions to $F_a^{(3)}$ with massive quark loop computed in [Chen, Czakon, Niggetiedt 2021]

Why numerical?

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



- 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

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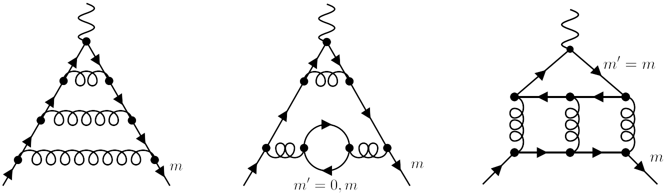
Setup



	nonsinglet	n_h-singlet
diagrams	271	66
families	34	17
integrals	302671	106883
masters	422	316

- 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 $\hat{s}$ with `LiteRed` [Lee 2012 + 2013]

Algorithm to solve master integrals

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

- Compute expansion around $\hat{s} = 0$ by:
  - Inserting an ansatz for the master integrals into the differential equation:

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

  - Compare coefficients in ϵ and $\hat{s}$ to establish linear system of equations for $c_{ij}^{(n)}$
  - Solve system in terms of small number of boundary constants using `Kira` with `FireFly` [Klappert, **FL** 2019; Klappert, Klein, **FL** 2020]
- Compute boundary values for $\hat{s} = 0$ to fix remaining constants

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- Compute boundary values for $\hat{s} = 0$ to fix remaining constants
- Construct expansion around new point $\hat{s} = \hat{s}_0$ by modifying the ansatz and repeating the steps above
- Match both expansions numerically at a point where both expansions converge, e.g. $\hat{s}_0/2$
- Repeat

Series expansions

- Different ansätze for different points:

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

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Series expansions

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

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

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

Series expansions

- Different ansätze for different points:

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

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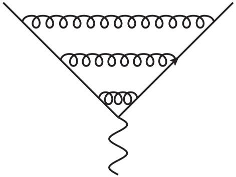
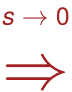
- We construct expansions up to $j_{\max} = 50$ around

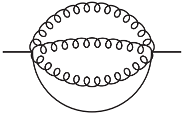
$$\hat{s} = \{-\infty, -32, -28, -24, -16, -12, -8, -4, 0, 1, 2, 5/2, 3, 7/2, 4, 9/2, 5, 6, 7, 8, 10, 12, 14, 15, 16, 17, 19, 22, 28, 40\}$$

and similar for the n_h-singlet contributions

Calculation of boundary conditions: nonsinglet







- For $s = 0$ the master integrals reduce to 3-loop on-shell propagators:
  - Well studied in the literature [Laporta, Remiddi 1996; Melnikov, van Ritbergen 1999; Lee, Smirnov 2010]
  - The reduction introduces high inverse powers in ϵ which requires some integrals up to weight 9
  - Using the dimensional-recurrence relations from [Lee, Smirnov 2010] we calculated the missing terms with `SummerTime.m` [Lee, Mingulov 2015] and `PSLQ` [Ferguson, Bailey, Arno 1999]

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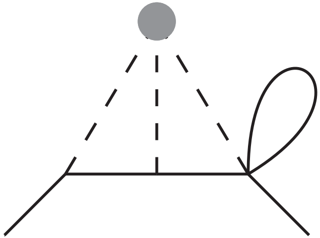
Calculation of boundary conditions: n_h singlet



- Due to massless cuts we need an asymptotic expansion
- Hard region solved with the same methods as in nonsinglet case
- Other regions:
  - Scalings identified with `asy.m` [Jantzen, Smirnov, Smirnov 2012]
  - α parameters integrated directly or with `HyperInt` [Panzer 2014]

$$J_3 = y^{-4\epsilon}\frac{\Gamma(\epsilon-1)\Gamma(2\epsilon)}{2}\int_0^\infty \mathrm{d}\alpha_3 \int_0^\infty \mathrm{d}\alpha_4 \int_0^\infty \mathrm{d}\alpha_6 \frac{\alpha_4^{-2\epsilon}\,\alpha_6^{-2\epsilon}\,(\alpha_6+\alpha_4(1+\alpha_6))^{3\epsilon-1}}{\alpha_4+\alpha_6+2\alpha_3\alpha_6+\alpha_3^2(1+\alpha_6)}$$

$$= y^{-4\epsilon}\pi^2 e^{-3\gamma_E\epsilon}\left\{-\frac{1}{6\epsilon^2}-\frac{7}{6\epsilon}+\frac{13\pi^2}{72}-\frac{43}{6}+\epsilon\left(\frac{59\zeta_3}{6}-\frac{259}{6}+\frac{91\pi^2}{72}\right)+\mathcal{O}(\epsilon^2)\right\}$$

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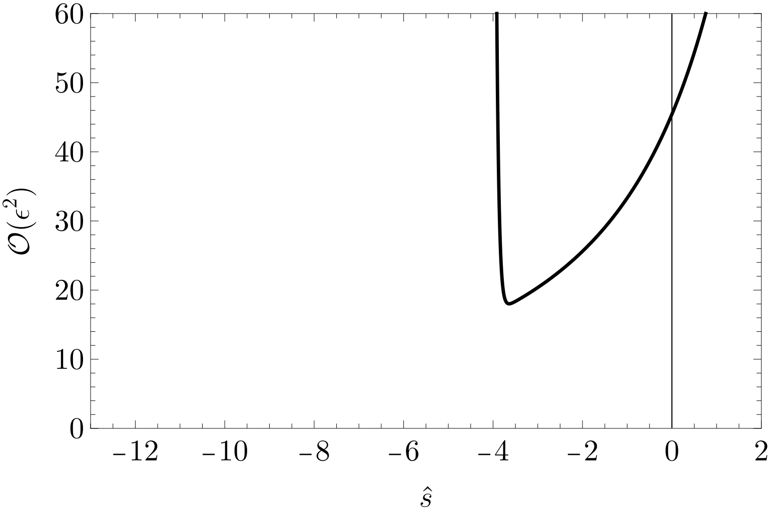
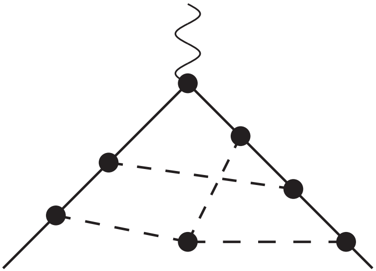
Example





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

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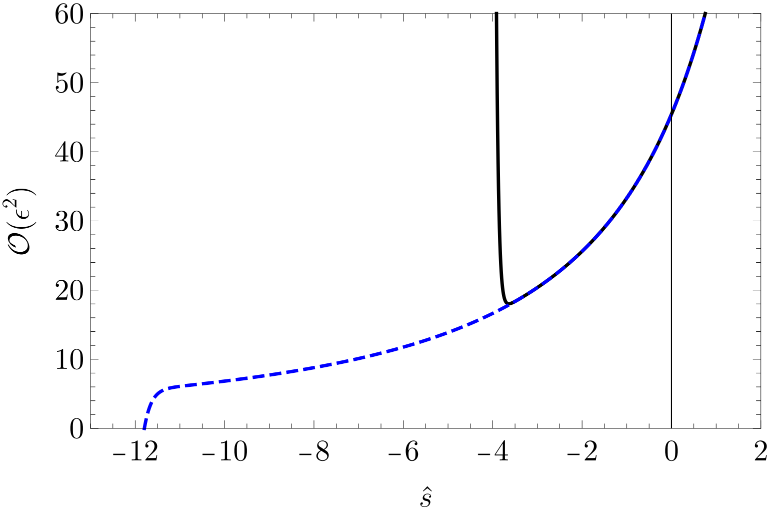

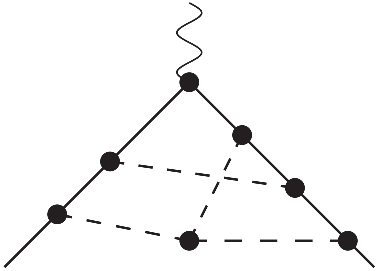

- Expansion around $\hat{s} = 0$
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$

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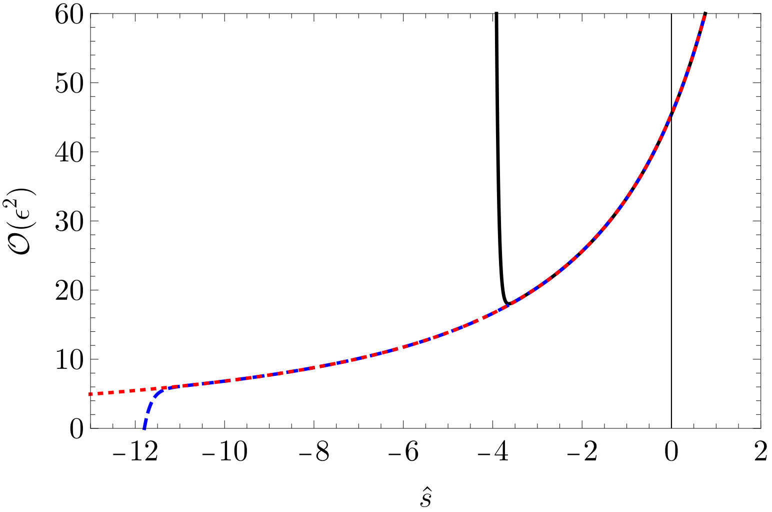

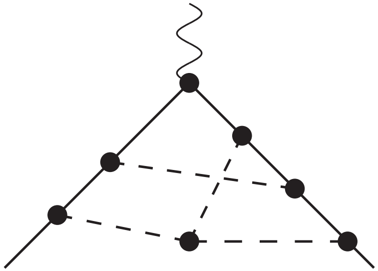

- Expansion around $\hat{s} = 0$
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$
- Expansion around $\hat{s} = -8$, matched at $\hat{s} = -6$

Similar algorithms in the literature

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Other approaches based on differential equations and series expansions:

- `SolveCoupledSystems.m` [Blümlein, Schneider 2017]
- `DESS.m` [Lee, Smirnov, Smirnov 2017]
- `DiffExp.m` [Hidding 2020] ⇒ Martijn Hidding's talk
- `AMFlow` [Liu, Ma 2022]
- `SeaSyde.m` [Armadillo, Bonciani, Devoto, Rana, Vicini 2022]
- ...

Our approach ...

- ... is tailored to problems with one real-valued kinematic variable
- ... does not require a special form for differential equations (except to be almost pole free on the diagonal)
- ... provides approximations over the whole kinematic range
- ... was successfully applied to physical quantities with 339, 422, and 316 master integrals [Fael, **FL**, Schönwald, Steinhauser 2021 + 2022]

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Renormalization and infrared structure

UV renormalization

- $\overline{\text{MS}}$ renormalization of α_s
- On-shell renormalization of mass Z_m^{OS}, wave function Z_2^{OS}, and (if needed) currents [Chetyrkin, Steinhauser 1999; Melnikov, van Ritbergen 2000]

IR subtraction

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

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

$$
\begin{aligned}
F_1^{\mathrm{v,f,(3)}}(\hat{s}=0) = \Bigg\{ & C_F^3 \bigg(-15 a_4 - \frac{17\pi^2\zeta_3}{24} - \frac{18367\zeta_3}{1728} + \frac{25\zeta_5}{8} - \frac{5 l_2^4}{8} - \frac{19}{40}\pi^2 l_2^2 + \frac{4957\pi^2 l_2}{720} + \frac{3037\pi^4}{25920} \\
& - \frac{24463\pi^2}{7776} + \frac{13135}{20736} \bigg) + C_A C_F^2 \bigg(\frac{19 a_4}{2} - \frac{\pi^2\zeta_3}{9} + \frac{17725\zeta_3}{3456} - \frac{55\zeta_5}{32} + \frac{19 l_2^4}{48} - \frac{97}{720}\pi^2 l_2^2 \\
& + \frac{29\pi^2 l_2}{240} - \frac{347\pi^4}{17280} - \frac{4829\pi^2}{10368} + \frac{707}{288} \bigg) + C_A^2 C_F \bigg(-a_4 + \frac{7\pi^2\zeta_3}{96} + \frac{4045\zeta_3}{5184} - \frac{5\zeta_5}{64} - \frac{l_2^4}{24} \\
& + \frac{67}{360}\pi^2 l_2^2 - \frac{5131\pi^2 l_2}{2880} + \frac{67\pi^4}{8640} + \frac{172285\pi^2}{186624} - \frac{7876}{2187} \bigg) \Bigg\} \hat{s} + \text{fermionic corrections} + \mathcal{O}(\hat{s}^2)
\end{aligned}
$$

- $l_2 = \ln(2)$, $a_4 = \mathrm{Li}_4(1/2)$ and $C_A = 3$, $C_F = 4/3$ for QCD
- Expansions for all currents are available up to $\mathcal{O}(\hat{s}^{67})$

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Results – high-energy limit

$$
\begin{aligned}
F_1^{\mathrm{v,f},(3)}\Big|_{s\to-\infty} &= 4.7318 C_F^3 - 20.762 C_F^2 C_A + 8.3501 C_F C_A^2 + \Big[3.4586 C_F^3 - 4.0082 C_F^2 C_A - 6.3561 C_F C_A^2\Big] l_s \\
&+ \Big[1.4025 C_F^3 + 0.51078 C_F^2 C_A - 2.2488 C_F C_A^2\Big] l_s^2 + \Big[0.062184 C_F^3 + 0.90267 C_F^2 C_A - 0.42778 C_F C_A^2\Big] l_s^3 \\
&+ \Big[-0.075860 C_F^3 + 0.20814 C_F^2 C_A - 0.035011 C_F C_A^2\Big] l_s^4 + \Big[-0.023438 C_F^3 + 0.019097 C_F^2 C_A\Big] l_s^5 \\
&+ \boxed{\Big[-0.0026042 C_F^3\Big] l_s^6} - \Big\{ -92.918 C_F^3 + 123.65 C_F^2 C_A - 47.821 C_F C_A^2 + \Big[-10.381 C_F^3 + 2.3223 C_F^2 C_A \\
&+ 17.305 C_F C_A^2\Big] l_s + \Big[4.9856 C_F^3 - 19.097 C_F^2 C_A + 8.0183 C_F C_A^2\Big] l_s^2 + \Big[3.0499 C_F^3 - 6.8519 C_F^2 C_A + 1.9149 C_F C_A^2\Big] l_s^3 \\
&+ \Big[0.67172 C_F^3 - 0.91213 C_F^2 C_A + 0.24069 C_F C_A^2\Big] l_s^4 + \Big[0.13229 C_F^3 - 0.051389 C_F^2 C_A + 0.0043403 C_F C_A^2\Big] l_s^5 \\
&+ \boxed{\Big[0.0041667 C_F^3 - 0.0010417 C_F^2 C_A - 0.00052083 C_F C_A^2\Big] l_s^6} \Big\} \frac{m^2}{s} + \mathcal{O}\left(\frac{m^4}{s^2}\right) + \text{fermionic contributions}
\end{aligned}
$$

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

$$
F_1^{\mathrm{v,f},(3)} = -\frac{C_F^3}{384} l_s^6 - \frac{m^2}{s}\left(\frac{C_F^3}{240} - \frac{C_F^2 C_A}{960} - \frac{C_F C_A^2}{1920}\right) l_s^6 + \ldots, \quad \text{with } l_s = \ln\left(\frac{m^2}{-s}\right)
$$

- We reproduce these terms with high precision

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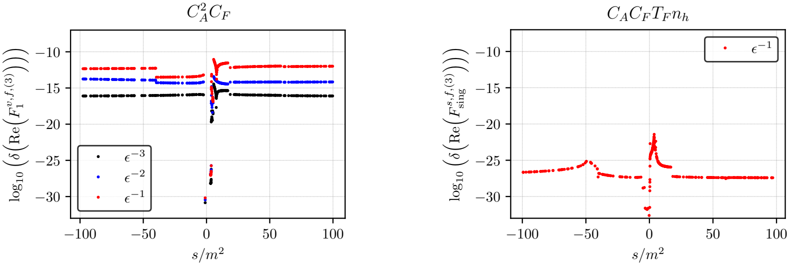
Results – pole cancellation

- 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

- Most regions for most color factors and especially n_h singlet much more precise



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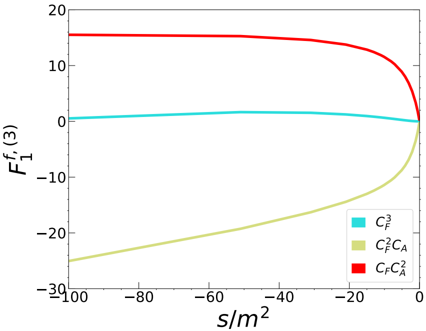
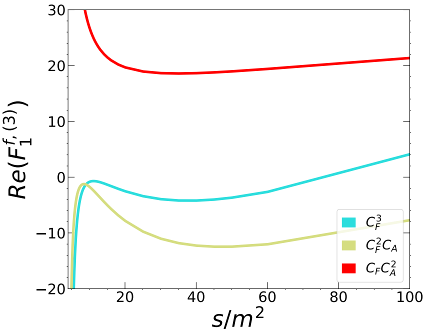
Results – some plots: nonsinglet





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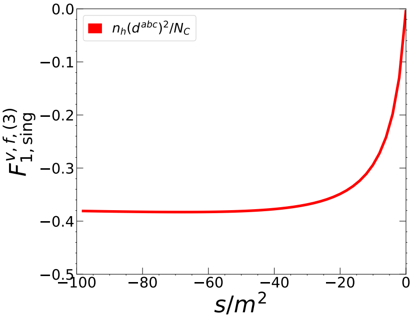
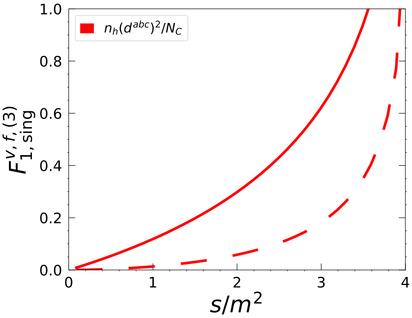
Results – some plots: n_h singlet





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

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

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

  with the quark velocity $\beta = \sqrt{1 - 4m^2/s}$
- Real radiation suppressed by β^3

$\Rightarrow$ Direct phenomenological relevance

- We find (with $l_{2\beta} = \ln(2\beta)$)

$$\begin{aligned}\Delta^{v,(3)} = {} & C_F^3 \left[-\frac{32.470}{\beta^2} + \frac{1}{\beta}\left(14.998 - 32.470 l_{2\beta}\right)\right] + C_A^2 C_F \frac{1}{\beta}\left[16.586 l_{2\beta}^2 - 22.572 l_{2\beta} + 42.936\right] \\ & + C_A C_F^2 \left[\frac{1}{\beta^2}\left(-29.764 l_{2\beta} - 7.7703\right) + \frac{1}{\beta}\left(-12.516 l_{2\beta} - 11.435\right)\right] \\ & + \mathcal{O}(\beta^0) + \text{fermionic contributions}\end{aligned}$$

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

Conclusions and outlook

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- Calculated nonsinglet and n_h-singlet contributions to massive quark form factors at NNNLO in QCD
- Applied a semianalytic method by constructing series expansions and matching numerically
- Reproduce known results from the literature, e.g.
  - large-N_c limit, n_l and partial n_h contributions
  - static, high-energy, and threshold expansions
- Estimate precision to at least 8 significant digits over the whole real axis
- Extracted matching coefficients between QCD and NRQCD [Egner, Fael, **FL**, Schönwald, Steinhauser 2022]

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Conclusions

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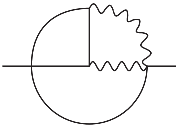
Outlook

- n_l-singlet contributions work in progress
- Singlet contributions to NRQCD matching coefficients
- $\gamma^\star \to \ell\bar{\ell}$ in QED most realistic first phenomenological application $\Rightarrow$ talks by Fulvio Piccinini and Yannick Ulrich

Calculation of Boundary Conditions

E.g. extension of G_{66} (given up to and including $\mathcal{O}(\epsilon^3)$ in [Lee, Smirnov 2010]):



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

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

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

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

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

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 $\{x_{k-1}, x_k, x_{k+1}\} \to \{-1, 0, 1\}$.