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# Singlet and non-singlet three-loop massive form factors

13th International Workshop on $e^+ e^-$ Collisions from $\Phi$ to $\Psi$

Kay Schönwald | Shanhai, August 19, 2022

TTP KARLSRUHE

[based on: Fael, Lange, Schönwald, Steinhauser, Phys. Rev. Lett. 128 (2022) and arxiv:2207.00027
Egner, Fael, Lange, Schönwald, Steinhauser, Phys. Rev. D 105 (2022)]

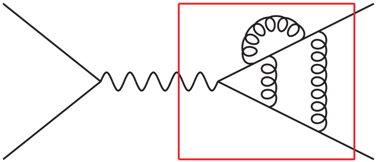
Institute for Theoretical Particle Physics

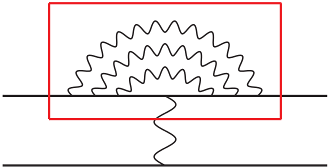
TRR 257 - Particle Physics Phenomenology after the Higgs Discovery

# Outline

# 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.

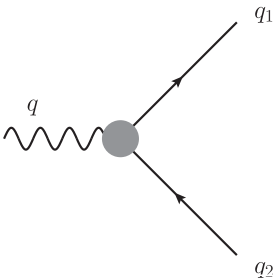




# The Process

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

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




vector : $j_\mu^v = \overline{\psi}\gamma_\mu\psi \qquad \Gamma_\mu^v = F_1^v(s)\gamma_\mu - \frac{i}{2m}F_2^v(s)\sigma_{\mu\nu}q^\nu$

axial-vector : $j_\mu^a = \overline{\psi}\gamma_\mu\gamma_5\psi \qquad \Gamma_\mu^a = F_1^a(s)\gamma_\mu\gamma_5 - \frac{1}{2m}F_2^a(s)q_\mu\gamma_5$

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

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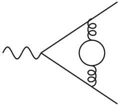
## NNLO

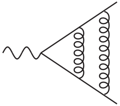
$F_l^{(2)}$ fermionic corrections [Hoang, Teubner '97]

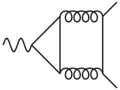


$F_l^{(2)}$ [Bernreuther, Bonciani, Gehrmann, Heinesch, Leineweber, Mastrolia, Remiddi '04-'06]

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

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



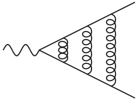


## NNNLO

$F_l^{(3)}$ 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]



this talk: full (numerical) results for non-singlet and singlet diagrams at NNNLO

# Previous Calculations

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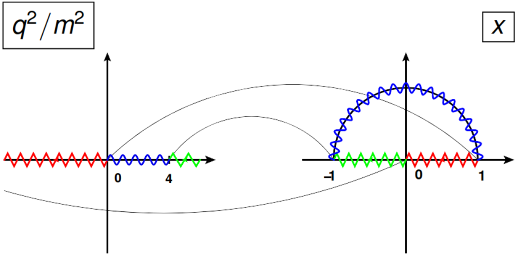
$$q^2 = s = -\frac{(1-x)^2}{x}$$



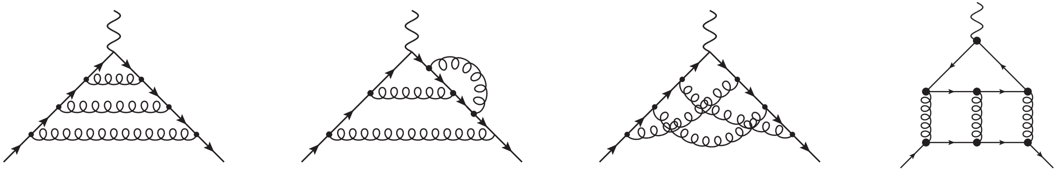

- The large-$N_c$ and $n_l$ contributions at NNLO can be written as iterated integrals over the letters:

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

- 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



- 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`. [Harlnder, 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 $\epsilon$ and $\hat{s}$ with `ImproveMasters.m`. [Smirnov, Smirnov '20]
- Establish differential equations in variable $\hat{s}$ using `LiteRed`. [Lee '12,'14]

| | non-singlet | singlet |
|---|---|---|
| diagrams | 271 | 66 |
| families | 34 | 17 |
| masters | 422 | 316 |

# Algorithm to Solve Master Integrals

- Establish a system of differential equations for the master integrals in the variable $\hat{s}$.
- Compute an expansion around $\hat{s} = 0$ by:
  - Inserting an ansatz for the master integrals into the differential equation.

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

  - Compare coefficients in $\epsilon$ and $\hat{s}$ to establish a linear system of equations for the $c_{ij}^{(n)}$.
  - Solve the linear system in terms of a small number of boundary constants using `Kira` with `FireFly`. [Klappert, Klein, Lange '19,'20]
- Compute boundary values for $\hat{s} = 0$ and obtain an analytic expansion.
- Build a general expansion around a new point, e.g. $\hat{s} = \hat{s}_0$, 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 the procedure for the next point.

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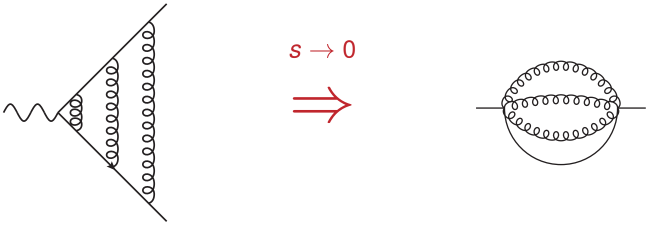
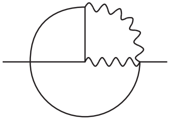
# Calculation of Boundary Conditions




- 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 $\epsilon$, which require some integrals up to weight 9.
- We calculate the needed terms with `SummerTime.m` [Lee, Mingulov '15] and `PSLQ` [Ferguson, Bailey '92].
- The singlet master integrals need a proper asymptotic expansion around $s = 0$, which we implemented with the help of `Asy.m` [Jantzen, Smirnov, Smirnov '12].

# Calculation of Boundary Conditions

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



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

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

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

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

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

# Series Expansions

- Special points:

| | | |
|---|---|---|
| $s = 0$ | $s = 4m^2$ | $s = \pm\infty$ |
| $x = 1$ | $x = -1$ | $x = 0$ |
| static limit | 2-particle threshold | high energy limit |

- Every expansion point needs a different ansatz:

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

# Series Expansions

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| | | |
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- Every expansion point needs a different ansatz:

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

# Series Expansions

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- Special points:

| | | |
|---|---|---|
| $s = 0$ | $s = 4m^2$ | $s = \pm\infty$ |
| $x = 1$ | $x = -1$ | $x = 0$ |
| static limit | 2-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:

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

- Every expansion point needs a different ansatz:

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

# Series Expansions

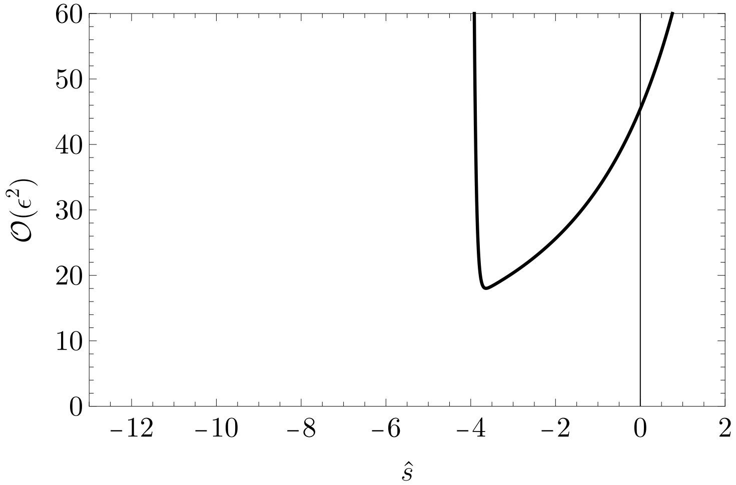
- Special points:

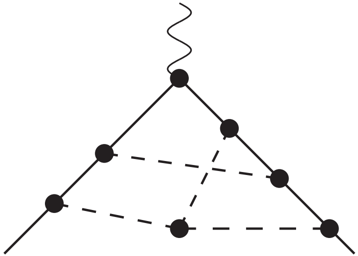
| $s = 0$ | $s = 4m^2$ | $s = \pm\infty$ | $s = 16m^2$ |
|---|---|---|---|
| $x = 1$ | $x = -1$ | $x = 0$ | $x = 4\sqrt{3} - 7$ |
| static limit | 2-particle threshold | high energy limit | 4-particle threshold |

- Every expansion point needs a different ansatz.
- We construct expansions with $j_{\max} = 50$ around:

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

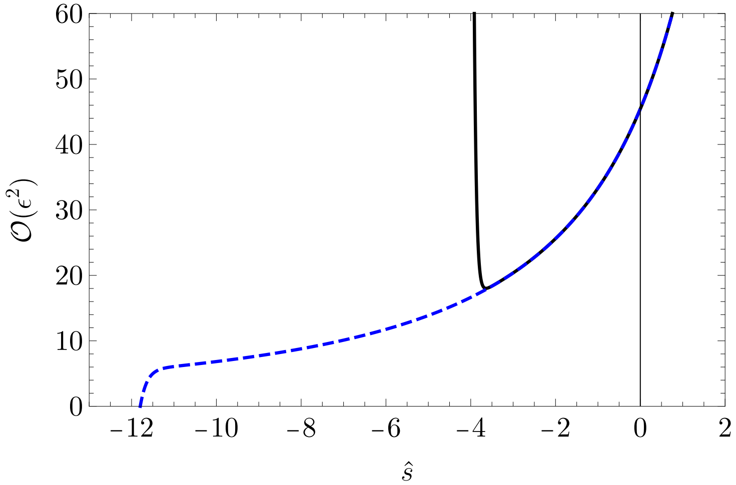
# Example

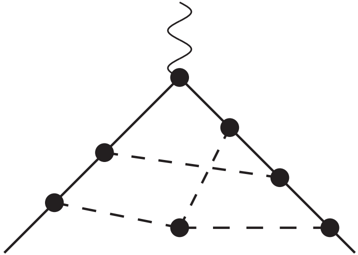


- Expansion around $\hat{s} = 0$.

# Example



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

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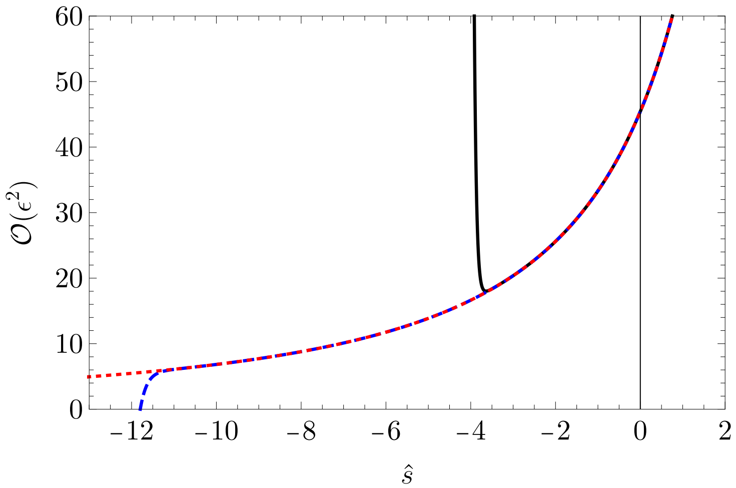


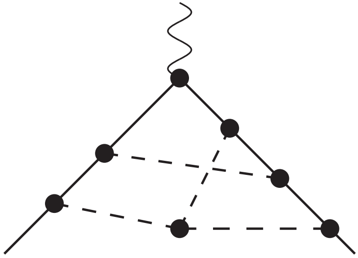

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- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$.
- Expansion around $\hat{s} = -8$, matched at $\hat{s} = -6$.

# 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]
- `AMFlow.m` [Liu, Ma '22]
- `SeaSyde.m` [Armadillo et al '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 $Z_m^{\mathrm{OS}}$, wave function $Z_2^{\mathrm{OS}}$, 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 $\Gamma_{\mathrm{cusp}}$.
  [Grozin, Henn, Korchemski, Marquard '14]
- Define finite form factors $F = Z_{\mathrm{IR}} F^{\mathrm{finite}}$ with the UV renormalized form factor $F$ and

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

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

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

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Analytic expansions for $\hat{s} = 0$:

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

with $l_2 = \ln(2)$, $a_4 = \mathrm{Li}_4(1/2)$ and $C_A = 3$, $C_F = 4/3$ for QCD.

- The expansions for all currents are available.
- We have calculated the expansion up to $\mathcal{O}(s^{67})$.

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

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# Results – Pole Cancellation

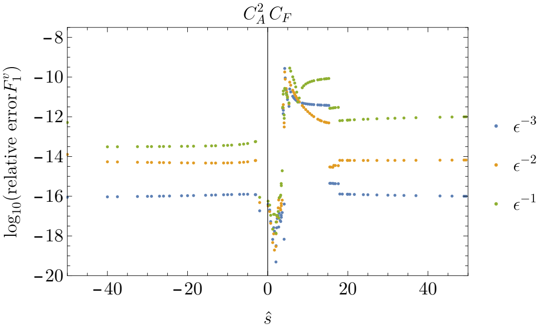
- Except for $s = 0$ the results of the expansions are not analytic.
- We can use the pole cancellation to estimate the precision.

$\Rightarrow$ We find at least 8 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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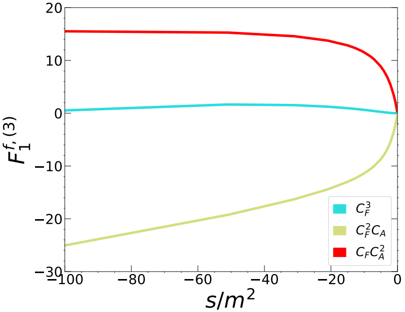


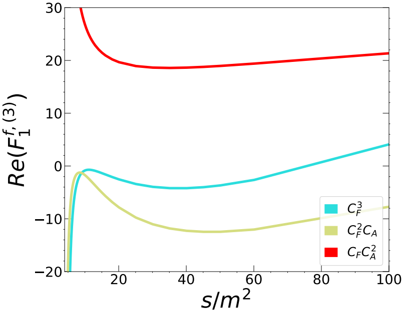

# Results – High Energy Limit

- For $s \to \infty$ there is the prediction: [Liu, Penin, Zerf '17]

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

- We obtain for example:

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

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# Results – Matching Coefficients

- For $Q\overline{Q}$ production close to threshold it is advantageous to calculate the cross section in non-relativistic QCD (NRQCD).
- The naive expansion around the threshold of the form factor

$$x = \sqrt{4 - \hat{s}} = 0$$

defines the matching coefficients between QCD and NRQCD. [Pineda '11]

- At threshold the momenta can have different scalings: [Beneke, Smirnov '98]
  - hard (h): $k_0 \sim m,\ k_i \sim m$
  - potential (p): $k_0 \sim x^2 \cdot m,\ k_i \sim x \cdot m$
  - soft (s): $k_0 \sim x \cdot m,\ k_i \sim x \cdot m$
  - ultrasoft (u): $k_0 \sim x^2 \cdot m,\ k_i \sim x^2 \cdot m$

# Results – Matching Coefficients

- The previous calculation relied heavily on sector decomposition and numerical integration with FIESTA. [Marquard, Piclum, Seidel, Steinhauser '14]
- We can improve the precision significantly:

$$\boxed{c_V^{(3)} = C_F^3 c_{FFF} + C_F C_A^2 c_{FFA} + C_F C_A^2 c_{FAA} + \text{fermionic and singlet contributions}}$$

$$\begin{aligned} c^V_{FFF} &= \phantom{-}36.55(0.53) &\rightarrow&\quad 36.49486246 \\ c^V_{FFA} &= -188.10(0.83) &\rightarrow&\quad -188.0778417 \\ c^V_{FAA} &= -\ 97.81(0.38) &\rightarrow&\quad -97.73497327 \end{aligned}$$

- We calculated the matching coefficients for all four currents.
- Recently new dedicated calculation with increased precision and two mass corrections [Feng et al, arXiv:2208.04302] .

# Conclusions and Outlook

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- We have calculated the non-singlet and 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, e.g.
  - the large $N_c$ limit.
  - expansion terms in the static, high energy and threshold expansion.
- We estimate the precision to 8 significant digits over the whole real axis.
- The method is promising to tackle other one-scale problems.

## Outlook

- Calculate the contributions of the singlet diagrams where the current couples to massless quarks.

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# Backup

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

# 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 $\beta^3$.
- We find (with $l_{2\beta} = \ln(2\beta)$):

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