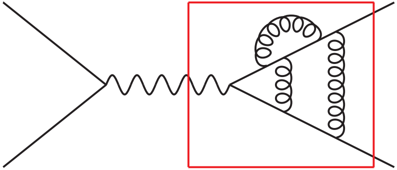
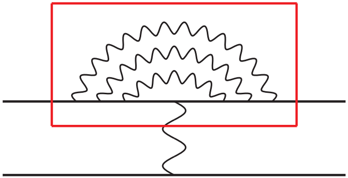
# Massive quark form factors at three loops

**Young Scientists Meeting of the CRC TRR 257 | June 8 – 10, 2022**

Fabian Lange
in collaboration with Matteo Fael, Kay Schönwald, Matthias Steinhauser | June 9, 2022

# 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 which is interesting to study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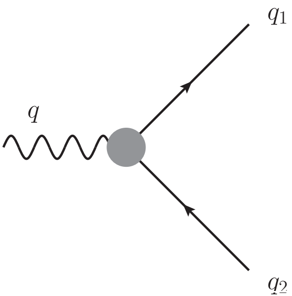
# The process



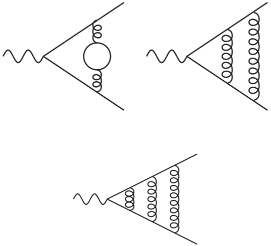

$$X(q) \to Q(q_1) + \bar{Q}(q_2)$$

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

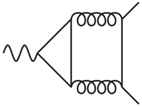
| | | |
|---|---|---|
| vector : | $j_\mu^{\mathrm{v}} = \overline{\psi}\gamma_\mu\psi,$ | $\Gamma_\mu^{\mathrm{v}} = F_1^{\mathrm{v}}(s)\gamma_\mu - \frac{\mathrm{i}}{2m}F_2^{\mathrm{v}}(s)\sigma_{\mu\nu}q^\nu$ |
| axial-vector : | $j_\mu^{\mathrm{a}} = \overline{\psi}\gamma_\mu\gamma_5\psi,$ | $\Gamma_\mu^{\mathrm{a}}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

# Status of massive non-singlet QCD corrections

non-singlet:



singlet:



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

- fermionic contributions [Hoang, Teubner 1997]
- complete [Bernreuther, Bonciani, Gehrmann, Heinesch, Leineweber, Mastrolia, Remiddi 2004 - 2005]

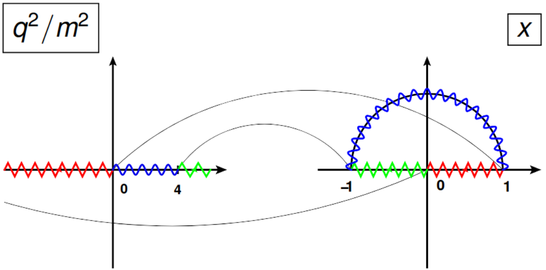
$F_i^{(3)}$ (**NNNLO**):

- 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]
- $n_l$ [Lee, Smirnov, Smirnov, Steinhauser 2018; Ablinger, Blümlein, Marquard, Rana, Schneider 2 $\times$ 2018]
- $n_h$ (partially) [Blümlein, Marquard, Rana, Schneider 2019]

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

# 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

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

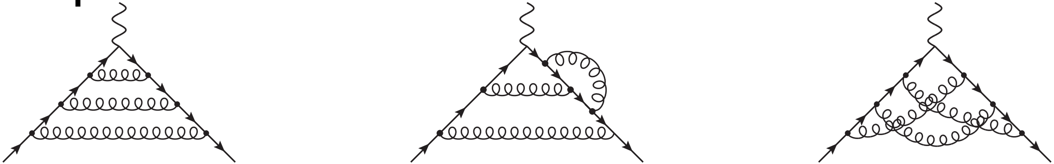
- $n_h$ terms already contain structures beyond iterated integrals (elliptic integrals)

$\Rightarrow$ No ready-to-use tools available for analytic solution

$\Rightarrow$ Instead: Full solution through analytic series expansions and numerical matching

# 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 $\epsilon$ and $\hat{s}$ with `ImproveMasters.m` [Smirnov, Smirnov 2020]
- Establish differential equations in $\hat{s}$ with `LiteRed` [Lee 2012 + 2013]

| | non-singlet |
|---|---|
| diagrams | 271 |
| families | 34 |
| integrals | 302671 |
| masters | 422 |

# Algorithm to solve master integrals

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

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

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

  - Compare coefficients in $\epsilon$ 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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  - 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
- 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 (including static limit at $s = 0$): $$M_n(\epsilon, \hat{s} = \hat{s}_0) = \sum_{i=-3}^{\infty} \sum_{j=0}^{j_{\max}} c_{ij}^{(n)} \, \epsilon^i \, (\hat{s} - \hat{s}_0)^j$$

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

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

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

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

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


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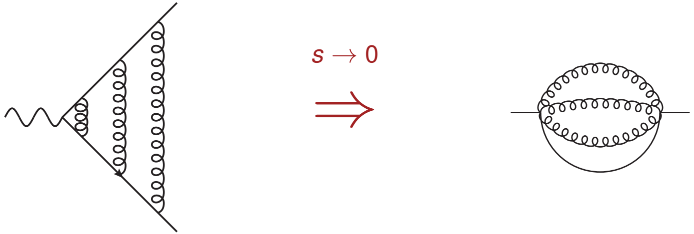
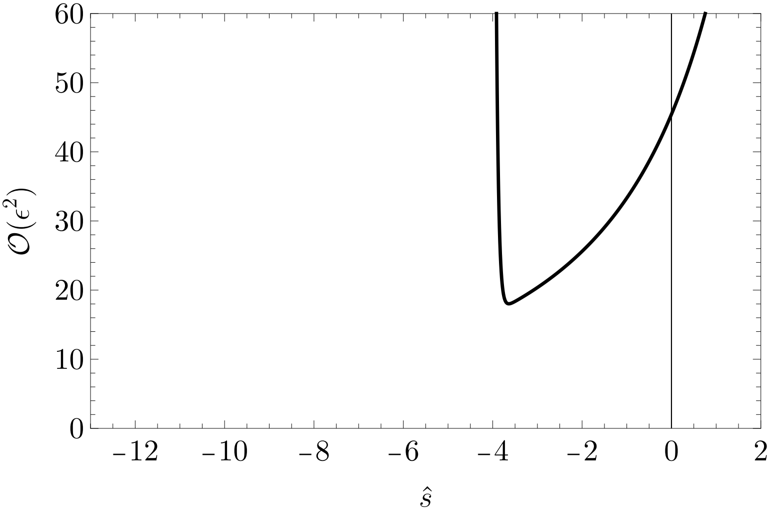
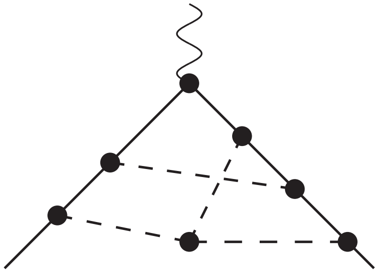
# Calculation of boundary conditions




- 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 $\epsilon$ 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]

# Example



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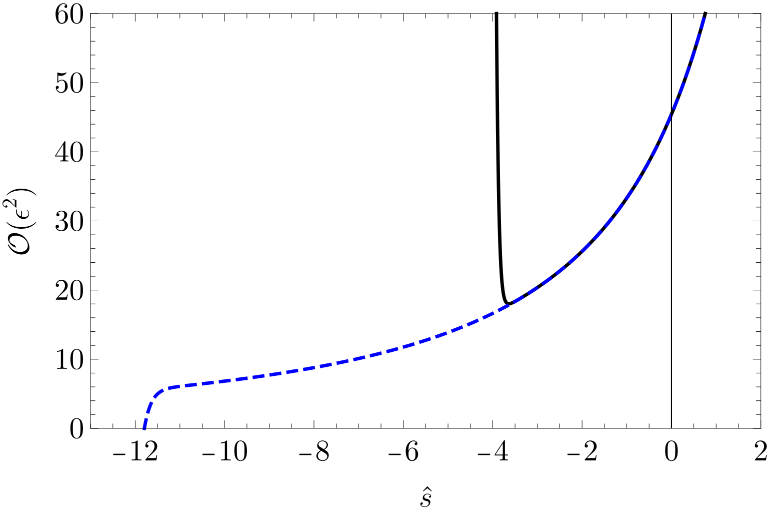
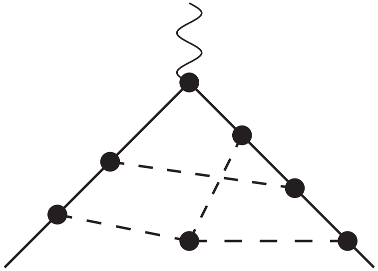
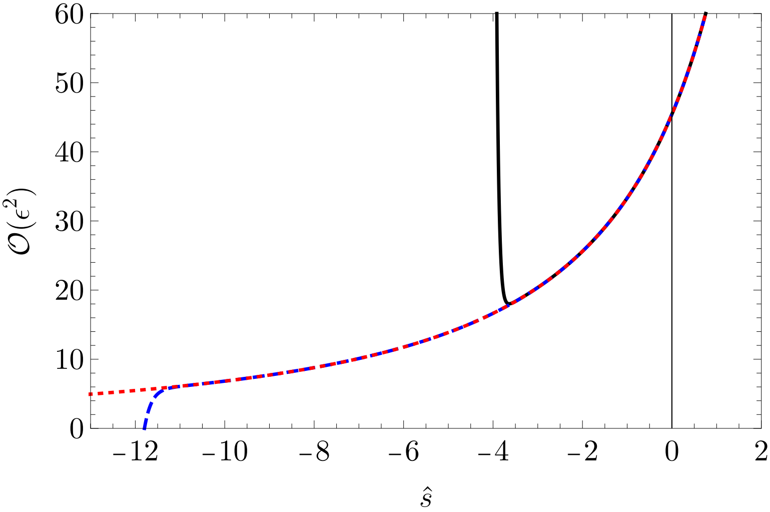
# Example

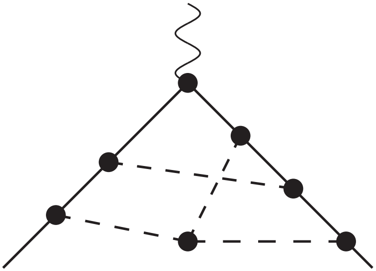


- Expansion around $\hat{s} = 0$
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$

# Example



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

# Similar algorithms in the literature

Other approaches based on differential equations and series expansions:

- `SolveCoupledSystems.m` [Blümlein, Schneider 2017]
- `DESS.m` [Lee, Smirnov, Smirnov 2017]
- `DiffExp.m` [Hidding 2020]
- `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 and 422 master integrals [Fael, **FL**, Schönwald, Steinhauser 2021 + 2022]

# Renormalization and infrared structure

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## UV renormalization

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

## IR subtraction

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

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

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

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

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

- $l_2 = \ln(2)$, $a_4 = \mathrm{Li}_4(1/2)$ 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] :

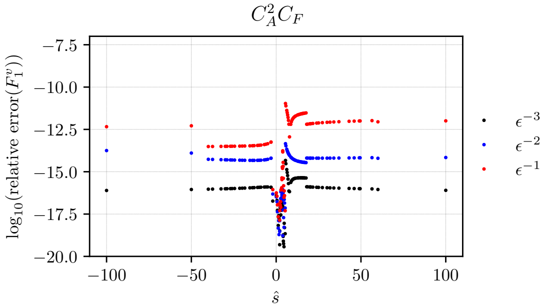
$$
F_1^{\mathrm{v,f},(3)} = -\frac{C_F^3}{384} l_s^6 - \frac{m^2}{s}\left(\frac{C_F^3}{240} - \frac{C_F^2 C_A}{960} - \frac{C_F C_A^2}{1920}\right) l_s^6 + \ldots, \quad \text{with } l_s = \ln\left(\frac{m^2}{-s}\right)
$$

- We reproduce these terms with high precision

# Results – pole cancellation

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

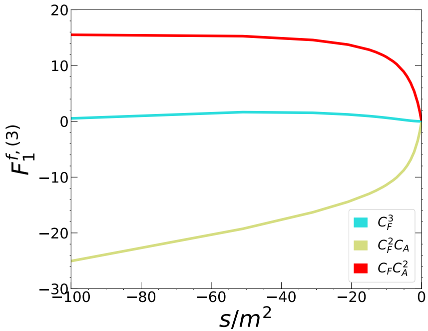
$$\log_{10}\left(\left|\frac{\text{expansion} - \text{analytic CT}}{\text{analytic CT}}\right|\right)$$

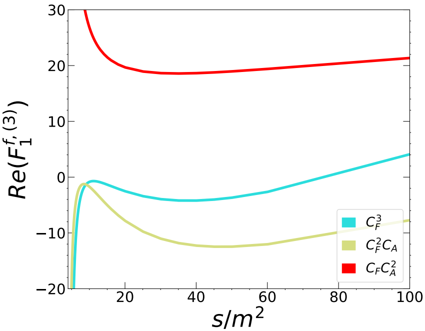



⇒ We estimate at least 8 correct digits for the finite terms

- Most regions much more precise

# Results – some plots



# 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 $\beta^3$

$\Rightarrow$ Direct phenomenological relevance

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

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

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

# Conclusions and outlook

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## Conclusions

- Calculated non-singlet contributions to massive quark form factors at NNNLO in QCD
  - Vector current partially published in [Fael, **FL**, Schönwald, Steinhauser 2022]
  - Other currents follow soon
- 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 $\Rightarrow$ talk by Manuel Egner

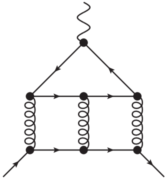
# Conclusions and outlook

## Conclusions

- Calculated non-singlet contributions to massive quark form factors at NNNLO in QCD
  - Vector current partially published in [Fael, **FL**, Schönwald, Steinhauser 2022]
  - Other currents follow soon
- 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 ⇒ talk by Manuel Egner

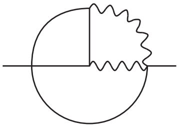
## Outlook

- Contributions of singlet diagrams
- Singlet contributions to NRQCD matching coefficients
- The method can be applied to other one-scale problems



# Calculation of Boundary Conditions

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



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

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

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

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

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



Institute for Theoretical Particle Physics and
Institute for Astroparticle Physics

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