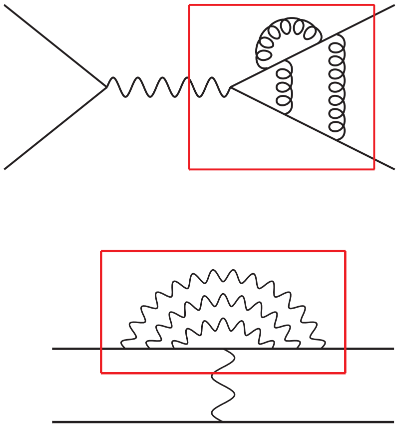
Massive quark form factors at three loops

LoopFest XX | May 12 – 14, 2022

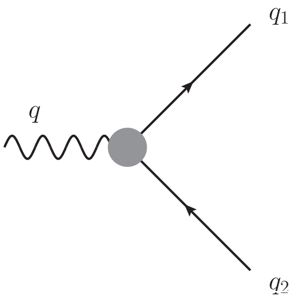
Fabian Lange
in collaboration with Matteo Fael, Kay Schönwald, Matthias Steinhauser | May 14, 2022

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

The process



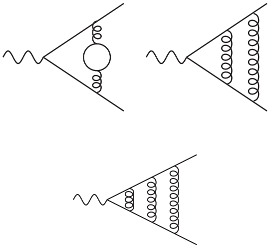
$$X(q) \to Q(q_1) + \bar{Q}(q_2)$$

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

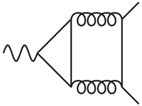
vector :	$j_\mu^{\mathrm{v}} = \overline{\psi}\gamma_\mu\psi,$	$\Gamma_\mu^{\mathrm{v}} = F_1^{\mathrm{v}}(s)\gamma_\mu - \frac{\mathrm{i}}{2m}F_2^{\mathrm{v}}(s)\sigma_{\mu\nu}q^\nu$
axial-vector :	$j_\mu^{\mathrm{a}} = \overline{\psi}\gamma_\mu\gamma_5\psi,$	$\Gamma_\mu^{\mathrm{a}} = F_1^{\mathrm{a}}(s)\gamma_\mu\gamma_5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

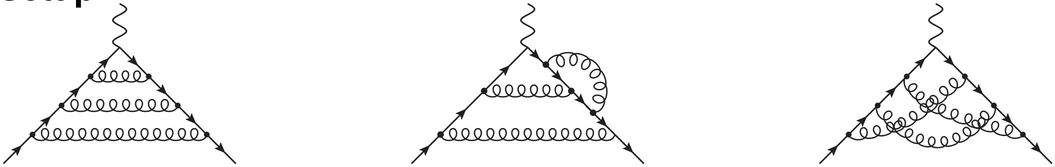
$F_i^{(3)}$ (**NNNLO**):

- 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

[see Andreas von Manteuffel's talk for four-loop massless form factors]

Setup



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

	non-singlet
diagrams	271
families	34
masters	422

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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 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

Algorithm to solve master integrals

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

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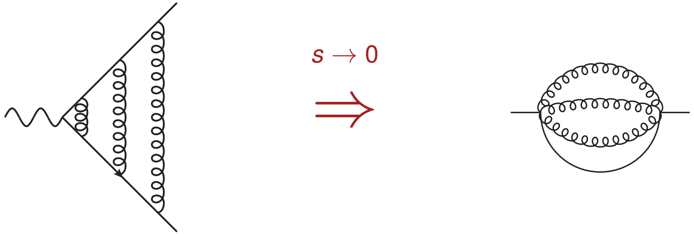
- We construct expansions up to $j_{\max} = 50$ around

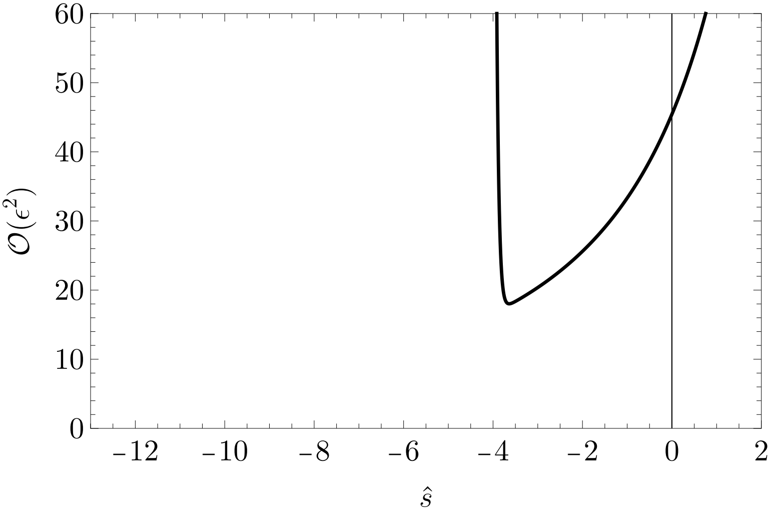
$$\hat{s} = \{-\infty, -32, -28, -24, -16, -12, -8, -4, 0, 1, 2, 5/2, 3, 7/2, 4, 9/2, 5, 6, 7, 8, 10, 12, 14, 15, 16, 17, 19, 22, 28, 40\}$$

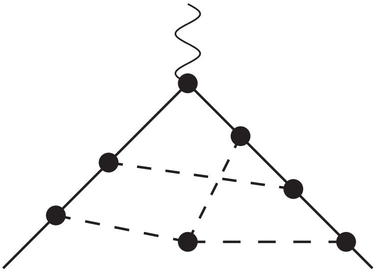
Calculation of boundary conditions



- 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 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]

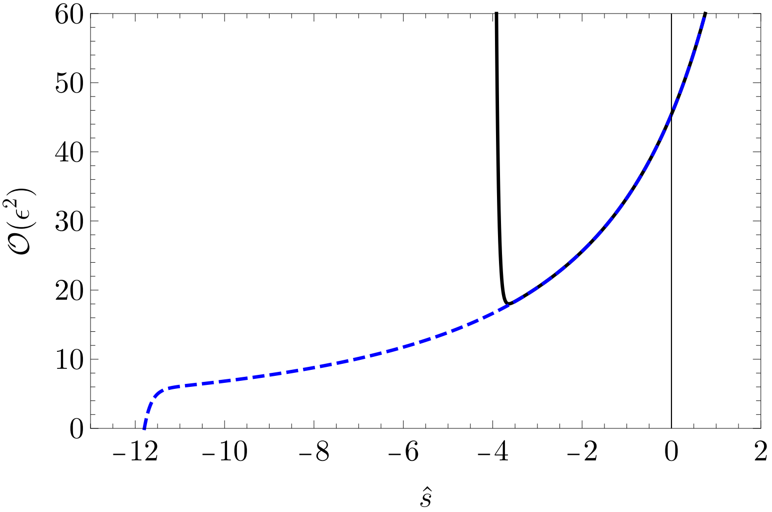
Example

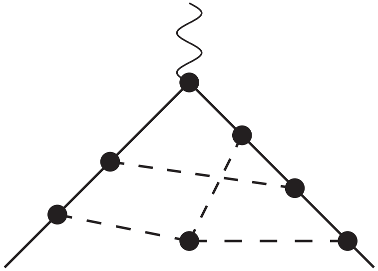




- Expansion around $\hat{s} = 0$

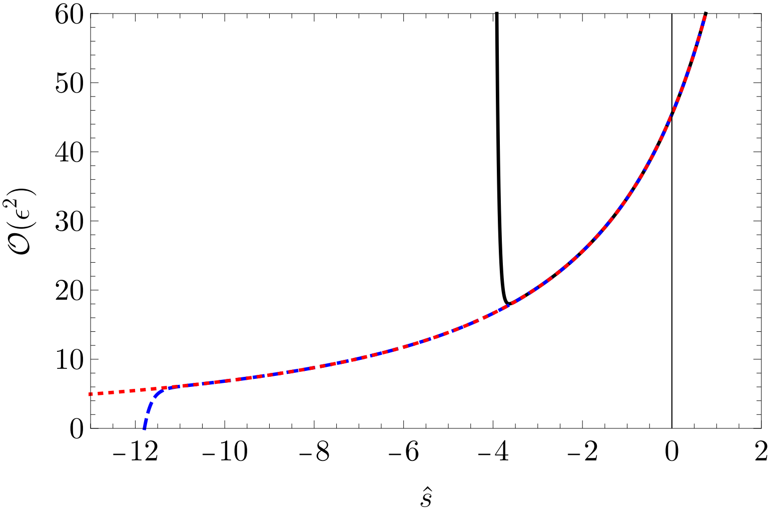
Example

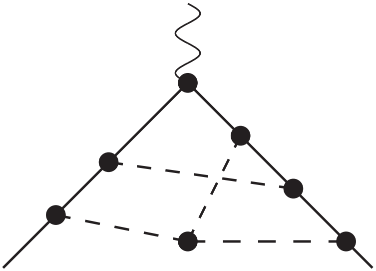




- Expansion around $\hat{s} = 0$
- Expansion around $\hat{s} = -4$, matched at $\hat{s} = -2$

Example





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

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]
- `SeaSyde.m` [Armadillo, Bonciani, Devoto, Rana, Vicini 2022] ⇐ talk by Alessandro Vicini
- `LoopTransport` ⇐ talk by Tobias Neumann
- ...

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]

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

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

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

Results – high-energy limit

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

- Prediction for leading logarithms [Liu, Penin, Zerf 2017] :

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

- We reproduce these terms with high precision

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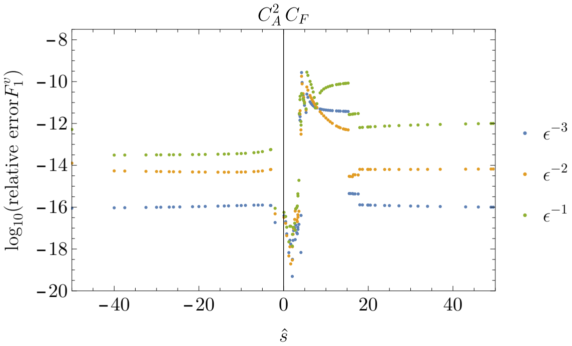
Results – pole cancellation

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

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

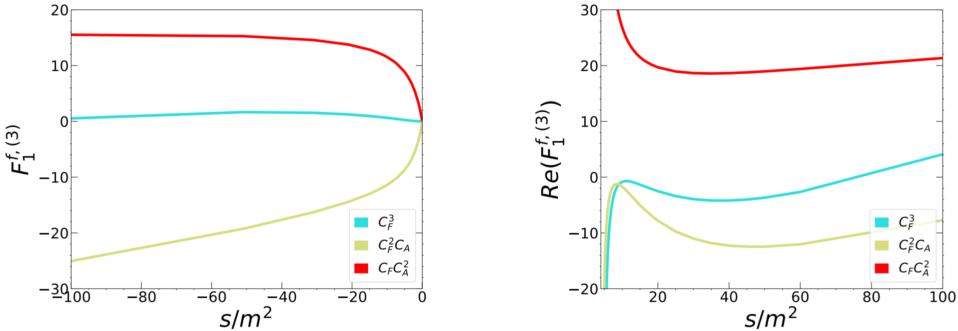
- Analytic expressions for poles expressed through harmonic polylogarithms which can be evaluated with `ginac` [Bauer, Frink, Kreckel 2000; Vollinga, Weinzierl 2005]



$\Rightarrow$ We estimate at least 8 correct digits for the finite terms

- All regions except the one between the thresholds much more precise

Results – some plots



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Conclusions and outlook

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Conclusions

- Calculated non-singlet contributions to massive quark form factors at NNLO in QCD
  - Vector current partially published in [Fael, **FL**, Schönwald, Steinhauser 2022]
  - Other currents soon
- Applied a semianalytic method by constructing series expansions and matching numerically
- Reproduce known results from the literature, e.g.
  - large-N_c limit
  - static, high-energy, and threshold expansions
- Estimate precision to 8 significant digits over the whole real axis
- Not shown: extracted matching coefficients between QCD and NRQCD [Egner, Fael, **FL**, Schönwald, Steinhauser 2022]

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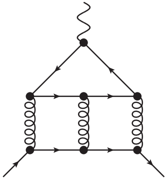
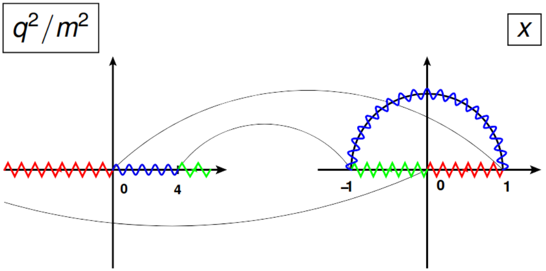
Outlook

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



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.

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Calculation of Boundary Conditions

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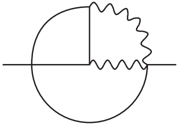
E.g. extension of G_{66} (given up to and including $\mathcal{O}(\epsilon^3)$ in [Lee, Smirnov 2010]):



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

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

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

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

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

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Moebius Transformations

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

Renormalization and infrared structure

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UV renormalization

- $\overline{\mathrm{MS}}$ 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 $F = Z_{\mathrm{IR}} F^{\mathrm{finite}}$ 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
- Γ_{cusp} universal for all currents

Results – Threshold Expansion

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- Close to threshold it is interesting to consider:

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

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

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

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

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

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

  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): $k_0 \sim x^2 \cdot m,\ k_i \sim x^2 \cdot m$

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Results – Matching Coefficients

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  - ultrasoft (u): $k_0 \sim x^2 \cdot m,\ k_i \sim x^2 \cdot m$
- We can obtain the matching coefficient by modifying the ansatz:

$$I_a \sim x^{-0\epsilon} \cdot \text{Taylor expansion} \quad (h-h-h)$$
$$I_b \sim x^{-2\epsilon} \cdot \text{Taylor expansion} \quad (h-h-p), (h-h-s), \ldots$$
$$I_c \sim x^{-4\epsilon} \cdot \text{Taylor expansion} \quad (h-h-u), (h-p-p), \ldots$$
$$I_d \sim x^{-6\epsilon} \cdot \text{Taylor expansion} \quad (h-p-u), (h-s-u), \ldots$$
$$I_e \sim x^{-8\epsilon} \cdot \text{Taylor expansion} \quad (h-u-u), (u-p-p), \ldots$$
$$I_f \sim x^{-10\epsilon} \cdot \text{Taylor expansion} \quad (u-u-p), (u-u-s)$$
$$I_g \sim x^{-12\epsilon} \cdot \text{Taylor expansion} \quad (u-u-u)$$

Results – Matching Coefficients

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

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

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

- We calculated the matching coefficients for all four currents.