B3: Perturbative QCD Results

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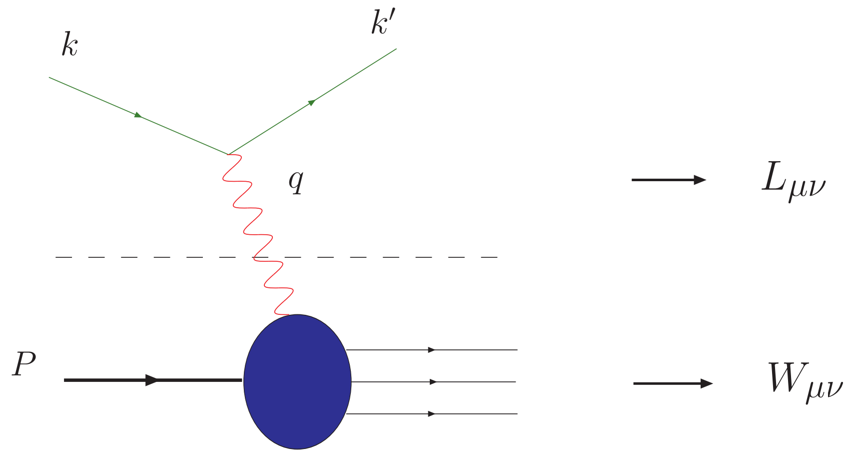
- Heavy Flavor Wilson Coefficients $O(a_s^3)$
- Polarized 3-loop Anomalous Dimensions
- General Unfolding of Moments

1. Heavy Flavor Wilson Coefficients to $O(a_s^3)$

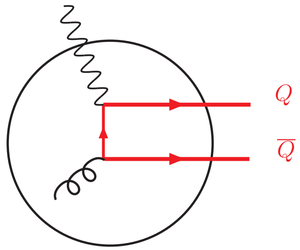
Deep–Inelastic Scattering (DIS):



$$Q^2 := -q^2, \quad x := \frac{Q^2}{2pq}$$ Bjorken–x

$$\frac{d\sigma}{dQ^2\, dx} \sim W_{\mu\nu} L^{\mu\nu}$$

LO:



Hadronic tensor for heavy quark production via single photon exchange:

$$W_{\mu\nu}^{Q\bar{Q}}(q,P,s) = \frac{1}{4\pi}\int d^4\xi \exp(iq\xi)\langle P,s \mid [J_\mu^{em}(\xi), J_\nu^{em}(0)] \mid P,s\rangle_{Q\bar{Q}}$$

unpol. $\left\{ \quad = \frac{1}{2x}\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) F_L^{Q\bar{Q}}(x,Q^2) + \frac{2x}{Q^2}\left(P_\mu P_\nu + \frac{q_\mu P_\nu + q_\nu P_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu}\right) F_2^{Q\bar{Q}}(x,Q^2)\right.$

pol. $\left\{ \quad -\frac{M}{2Pq}\varepsilon_{\mu\nu\alpha\beta} q^\alpha \left[s^\beta g_1^{Q\bar{Q}}(x,Q^2) + \left(s^\beta - \frac{sq}{Pq} p^\beta\right) g_2^{Q\bar{Q}}(x,Q^2)\right]\right. .$

- In the limit $Q^2 \gg m_Q^2$ [$Q^2 \approx 10\ m_Q^2$ for F_2]:
  massive RGE, derivative $m^2\partial/\partial m^2$ acts on Wilson coefficients only: all terms but power corrections calculable through partonic operator matrix elements, $\langle i|A_l|j\rangle$, which are process independent objects!

$$H_{(2,L),i}^{\rm S,NS}\left(\frac{Q^2}{\mu^2},\frac{m^2}{\mu^2}\right) = \underbrace{A_{k,i}^{\rm S,NS}\left(\frac{m^2}{\mu^2}\right)}_{\text{massive OMEs}} \otimes \underbrace{C_{(2,L),k}^{\rm S,NS}\left(\frac{Q^2}{\mu^2}\right)}_{\text{light–parton–Wilson coefficients}} .$$

- holds for polarized and unpolarized case. OMEs obey expansion

$$A_{k,i}^{\rm S,NS}\left(\frac{m^2}{\mu^2}\right) = \langle i|O_k^{\rm S,NS}|i\rangle = \delta_{k,i} + \sum_{l=1}^{\infty} a_s^l A_{k,i}^{{\rm S,NS},(l)}\left(\frac{m^2}{\mu^2}\right), \qquad i = q, g$$

[Buza, Matiounine, Migneron, Smith, van Neerven, 1996; Buza, Matiounine, Smith, van Neerven, 1997.]

- OMEs can be used in a variable–flavor–number–scheme to define a heavy quark density

$$f_{Q+\bar{Q}}(n_f+1,\mu^2) = \tilde{A}_{Qq}^{\rm PS}\left(n_f,\frac{\mu^2}{m^2}\right)\otimes \underbrace{\Sigma(n_f,\mu^2)}_{\text{Singlet density}} + \tilde{A}_{Qg}^{\rm S}\left(n_f,\frac{\mu^2}{m^2}\right)\otimes \underbrace{G(n_f,\mu^2)}_{\text{Gluon density}} .$$

[Buza, Matiounine, Smith, van Neerven, 1998]

Renormalization

$$\hat{\hat{A}}_{ij} = \delta_{ij} + \sum_{k=0}^{\infty} \hat{a}_s^k \hat{\hat{A}}_{ij}^{(k)}$$

- Mass renormalization (on–mass shell scheme)
- Charge renormalization

$\longrightarrow$ use $\overline{\text{MS}}$ scheme $(D = 4 + \varepsilon)$ working intermediarily in a MOM-scheme and apply the decoupling formalism [Ovrut, Schnitzer, 1981; Bernreuther, Wetzel, 1982].

- Renormalization of ultraviolet singularities
  $\Longrightarrow$ are absorbed into Z–factors given in terms of anomalous dimensions γ_{ij}.
- Factorization of collinear singularities
  $\Longrightarrow$ are factored into Γ–factors Γ_{NS}, $\Gamma_{ij,S}$ and $\Gamma_{qq,PS}$.
  For massless quarks it would hold: $\Gamma = Z^{-1}$.
  Here: Γ–matrices apply to parts of the diagrams with massless lines only .

Generic formula for operator renormalization and mass factorization:

$$A_{ij} = Z_{il}^{-1} \hat{A}_{lm} \Gamma_{mj}^{-1}$$

$\Longrightarrow$ $O(\varepsilon)$–terms of the 2–loop OMEs are needed for renormalization at 3–loops.

2–Loop Results

- Calculation in Mellin-space for space–like q^2 up to $O(\varepsilon)$.
- Summation of lots of new infinite one-parameter sums into harmonic sums. Use of integral techniques and the Mathematica package SIGMA [C. Schneider, 2007],
  [I. Bierenbaum, J. Blümlein, S. K., C. Schneider, 2007, 2008]
- We calculated all 2–loop $O(\varepsilon)$–terms in the unpolarized case:

$$\overline{a}_{Qg}^{(2)}, \quad \overline{a}_{Qq}^{(2),\mathbf{PS}}, \quad \overline{a}_{gg,Q}^{(2)}, \quad \overline{a}_{gq,Q}^{(2)}, \quad \overline{a}_{qq,Q}^{(2),\mathbf{NS}}.$$

- Mathematical structure of the $\mathrm{O}(\varepsilon)$ terms:

$$\{S_1, \ S_2, \ S_3, \ S_4, \ S_{-2}, S_{-3}, S_{-4}\}, \quad S_{2,1}, \quad S_{-2,1}, \quad S_{-3,1}, \quad S_{2,1,1}, \quad S_{-2,1,1}$$

  $\Longrightarrow$ 6 basic objects

- These objects are in common to all single scale higher order processes.
  Str. Functions, DIS HQ, Fragm. Functions, DY, Hadr. Higgs-Prod., s+v contr. to Bhabha scatt., ...
- harmonic sums with index $\{-1\}$ cancel (holds even for each diagram)
- Expectation for 3–loops: weight 5 (6) harmonic sums

Fixed moments at 3–Loop

Bierenbaum, Blümlein, Klein :

Contributing OMEs:

Singlet	A_{Qg}	$A_{qg,Q}$	$A_{gg,Q}$	$A_{gq,Q}$	} mixing
Pure–Singlet		$A_{Qq}^{\rm PS}$	$A_{qq,Q}^{\rm PS}$		
Non–Singlet	$A_{qq,Q}^{\rm NS,+}$	$A_{qq,Q}^{\rm NS,-}$	$A_{qq,Q}^{\rm NS,v}$		

- All 2–loop $O(\varepsilon)$–terms in the unpolarized case are known:
- Unpolarized anomalous dimensions are known up to $O(a_s^3)$ [Moch, Vermaseren, Vogt, 2004.]
  $\Longrightarrow$ All terms needed for the renormalization of unpolarized 3–Loop heavy OMEs are present.
  $\Longrightarrow$ Calculation will provide first independent checks on $\gamma_{qg}^{(3)}$, $\gamma_{qq}^{(3),\rm PS}$ and on respective color projections of $\gamma_{qq}^{(3),{\rm NS}\pm,{\rm v}}$, $\gamma_{gg}^{(3)}$ and $\gamma_{gq}^{(3)}$.
- Calculation proceeds in the same way in the polarized case. Known so far :

$$\Delta\overline{a}_{Qg}^{(2)}, \quad \Delta\overline{a}_{Qq}^{(2),\mathbf{PS}}, \quad \Delta\overline{a}_{qq,Q}^{(2),\mathbf{NS}} = \overline{a}_{qq,Q}^{(2),\mathbf{NS}} \; .$$

Fixed moments using MATAD

- three–loop "self-energy" type diagrams with an operator insertion
- Extension: additional scale compared to massive propagators: Mellin variable N
- Genuine tensor integrals due to

$$\Delta^{\mu_1}...\Delta^{\mu_n} \langle p|O_{\mu_1...\mu_n}|p\rangle = \Delta^{\mu_1}...\Delta^{\mu_n} \langle p|S\,\bar{\Psi}\gamma_{\mu_1}D_{\mu_2}...D_{\mu_n}\Psi|p\rangle = A(N)\cdot(\Delta p)^N$$

$$D_\mu = \partial_\mu - igt_a A_\mu^a \quad , \qquad \Delta^2 = 0.$$

- Construction of a projector to obtain the desired moment in N [undo Δ-contraction]
- 3–loop OMEs are generated with QGRAF [Nogueira, 1993]
- Color factors are calculated with [Ritbergen, Schellekens, Vermaseren, 1998]
- Translation to suitable input for MATAD [Steinhauser, 2001]

Tests performed:

- Various 2–loop calculations for $N = 2, 4, 6, ...$ were repeated
  $\longrightarrow$ agreement with our previous calculation.
- Several non–trivial scalar 3–loop diagrams were calculated using Feynman–parameters for all N
  $\longrightarrow$ agreement with MATAD.

General structure of the result: the PS –case

$$A_{Qq}^{(3),\mathrm{PS}} + A_{qq,Q}^{(3),\mathrm{PS}} = \frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{48}\left\{\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 4(n_f+1)\beta_{0,Q} + 6\beta_0\right\}\ln^3\left(\frac{m^2}{\mu^2}\right)$$

$$+\left\{\frac{\hat{\gamma}_{qq}^{(1),\mathrm{PS}}}{2}\Big((n_f+1)\beta_{0,Q} - \beta_0\Big) + \frac{\hat{\gamma}_{qg}^{(0)}}{8}\Big((n_f+1)\hat{\gamma}_{gq}^{(1)} - \gamma_{gq}^{(1)}\Big) - \frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}}{8}\right\}\ln^2\left(\frac{m^2}{\mu^2}\right)$$

$$+\left\{\frac{\hat{\gamma}_{qq}^{(2),\mathrm{PS}}}{2} - \zeta_2\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{16}\Big(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 4(n_f+1)\beta_{0,Q} + 6\beta_0\Big) - 2a_{Qq}^{(2),\mathrm{PS}}\beta_0\right.$$

$$\left.+\frac{n_f+1}{2}\hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)} - \frac{\gamma_{gq}^{(0)}}{2}a_{Qg}^{(2)}\right\}\ln\left(\frac{m^2}{\mu^2}\right) + \zeta_3\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}}{48}\Big(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 4n_f\beta_{0,Q} + 6\beta_0\Big)$$

$$+\frac{\zeta_2}{16}\Big(-4n_f\beta_{0,Q}\hat{\gamma}_{qq}^{(1),\mathrm{PS}} + \hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(1)}\Big) + 4(\beta_0 + \beta_{0,Q})\overline{a}_{Qq}^{(2),\mathrm{PS}} + \gamma_{gq}^{(0)}\overline{a}_{Qg}^{(2)} - (n_f+1)\hat{\gamma}_{qg}^{(0)}\overline{a}_{gq,Q}^{(2)}$$

$$+C_F\Big(-(4+\frac{3}{4}\zeta_2)\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)} - 4\hat{\gamma}_{qq}^{(1),\mathrm{PS}} + 12a_{Qq}^{(2),\mathrm{PS}}\Big) + a_{Qq}^{(3),\mathrm{PS}} + a_{qq,Q}^{(3),\mathrm{PS}}\ .$$

- n_f–dependence non–trivial. Take all quantities at n_f flavors and adopt notation

$$\hat{\gamma}_{ij} \equiv \gamma_{ij}(n_f+1) - \gamma_{ij}(n_f)\ , \quad \beta_{0,Q} \equiv \beta_0(n_f+1) - \beta_0(n_f)\ .$$

- We calculated the PS- and NS$^+$–terms for $N = 2, 4, 6, 8$ using MATAD and find agreement of the pole terms with the prediction obtained from renormalization.

Result for the renormalized PS–term for $N = 4$.

$$
\left. A_{Qq}^{(3),\mathrm{PS}} + A_{qq,Q}^{(3),\mathrm{PS}} \right|_{N=4} = \Biggl\{ -\frac{484}{2025} C_F {T_F}^2 (2n_f + 1) + \frac{4598}{3375} C_F C_A T_F - \frac{18997}{40500} {C_F}^2 T_F \Biggr\} \ln^3\left(\frac{m^2}{\mu^2}\right)
$$
$$
+ \Biggl\{ -\frac{16}{125} C_F {T_F}^2 + \frac{36751}{202500} C_F C_A T_F - \frac{697631}{405000} {C_F}^2 T_F \Biggr\} \ln^2\left(\frac{m^2}{\mu^2}\right) + \Biggl\{ -\frac{2131169}{303750} C_F {T_F}^2 n_f
$$
$$
- \frac{427141}{121500} C_F {T_F}^2 + \left(-\frac{484}{75} \zeta_3 + \frac{24888821}{2700000} \right) C_F C_A T_F + \left(\frac{484}{75} \zeta_3 + \frac{63582197}{16200000} \right) {C_F}^2 T_F \Biggr\} \ln\left(\frac{m^2}{\mu^2}\right)
$$
$$
+ \left(\frac{7744}{2025} \zeta_3 - \frac{143929913}{27337500} \right) C_F {T_F}^2 n_f + \left(-\frac{13552}{2025} \zeta_3 + \frac{218235943}{54675000} \right) C_F {T_F}^2 + \left(\frac{242}{225} \mathrm{B4} - \frac{242}{25} \zeta_4 \right.
$$
$$
\left. + \frac{86833}{13500} \zeta_3 + \frac{4628174}{1265625} \right) C_F C_A T_F + \left(-\frac{484}{225} \mathrm{B4} + \frac{242}{25} \zeta_4 + \frac{298363}{20250} \zeta_3 - \frac{57518389433}{2187000000} \right) {C_F}^2 T_F \ .
$$

- All terms proportional to ζ_2 have cancelled in the renormalized result.
- We observe a new number

$$
\mathrm{B4} \quad = \quad -4\zeta_2 \ln^2 2 + \frac{2}{3} \ln^4 2 - \frac{13}{2} \zeta_4 + 16 \mathrm{Li}_4\left(\frac{1}{2}\right) = -8\sigma_{-3,-1} + \frac{11}{2} \zeta_4 \ .
$$

- The term B4 appears as $T_F C_F (C_F - C_A/2) \mathrm{B4}$.
- B4 appeared in an observable first in 1994 (J. Fleischer et al.); 1996 (E. Remiddi et al.).
- Likely also $S_{-3,-1}(N)$ is there.

We obtain for the moments of the NS and PS anomalous dimenions

N	$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}/T_F/C_F$
2	$-\frac{5024}{243}T_F(1+2n_f)+\left(\frac{10136}{243}-\frac{256}{3}\zeta_3\right)C_A+\left(-\frac{14728}{243}+\frac{256}{3}\zeta_3\right)C_F$
4	$-\frac{618673}{151875}T_F(1+2n_f)+\left(\frac{2485097}{506250}-\frac{968}{75}\zeta_3\right)C_A+\left(-\frac{2217031}{675000}+\frac{968}{75}\zeta_3\right)C_F$
6	$-\frac{126223052}{72930375}T_F(1+2n_f)+\left(\frac{1988624681}{4084101000}-\frac{3872}{735}\zeta_3\right)C_A+\left(\frac{11602048711}{10210252500}+\frac{3872}{735}\zeta_3\right)C_F$
8	$-\frac{13131081443}{13502538000}T_F(1+2n_f)+\left(-\frac{343248329803}{648121824000}-\frac{2738}{945}\zeta_3\right)C_A+\left(\frac{39929737384469}{22684263840000}+\frac{2738}{945}\zeta_3\right)C_F$

N	$\hat{\gamma}_{qq}^{(2),\mathsf{NS},+}/T_F/C_F$
2	$-\frac{1792}{243}T_F(1+2n_f)-\left(\frac{256}{3}\zeta_3+\frac{12512}{243}\right)C_A+\left(\frac{256}{3}\zeta_3-\frac{13648}{243}\right)C_F$
4	$-\frac{384277}{30375}T_F(1+2n_f)-\left(\frac{2512}{15}\zeta_3+\frac{8802581}{121500}\right)C_A+\left(\frac{2512}{15}\zeta_3-\frac{165237563}{1215000}\right)C_F$
6	$-\frac{160695142}{10418625}T_F(1+2n_f)-\left(\frac{22688}{105}\zeta_3+\frac{13978373}{171500}\right)C_A+\left(\frac{22688}{105}\zeta_3-\frac{44644018231}{243101250}\right)C_F$
8	$-\frac{38920977797}{2250423000}T_F(1+2n_f)-\left(\frac{79064}{315}\zeta_3+\frac{1578915745223}{18003384000}\right)C_A+\left(\frac{79064}{315}\zeta_3-\frac{91675209372043}{420078960000}\right)C_F$

$\Longrightarrow$ Agreement for the terms $\propto\ T_F$ with

[Larin, Nogueira, Ritbergen, Vermaseren, 1997; Moch, Vermaseren, Vogt, 2004]

- also finished: $N = 10$
- currently running: $N = 12, 14$, $\quad$ NS$^+$, PS; $\quad A_{Qg}$
- preparing for: A_{gQ}, A_{gg}

$\Longrightarrow$ needed to establish the variable flavor scheme to 3-loops;

$\Longrightarrow$ PDF's at LHC

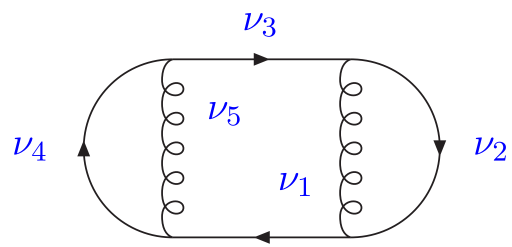
How far can we go with present technology ?

NS, PS: $N = 14$ requires 64 GB machines and 2-3 months run time;
likely to be the case for A_{Qg}, $N = 12$ ...

- `tform` is not always in harmony with `MATAD`, which would be important.

First General N Results at 3–Loop

Consider e.g the 3–loop tadpole diagram



Using Feynman–parameters, one obtains a representation in terms of a double sum

$$I_4 = C_4 \Gamma \left[\begin{matrix} 2+\varepsilon/2-\nu_1, 2+\varepsilon/2-\nu_5, \nu_{12}-2-\varepsilon/2, \nu_{45}-2-\varepsilon/2, \nu_{1345}-4-\varepsilon, \nu_{12345}-6-3/2\varepsilon \\ \nu_1, \nu_2, \nu_4, 2+\varepsilon/2, \nu_{345}-2-\varepsilon/2, \nu_{12345}-4-\varepsilon \end{matrix} \right]$$
$$\sum_{m,n=0}^{\infty} \frac{(\nu_{345}-2-\varepsilon/2)_{n+m}(\nu_{12345}-6-3/2\varepsilon)_m(2+\varepsilon/2-\nu_1)_m(2+\varepsilon/2-\nu_5)_n(\nu_{45}-2-\varepsilon/2)_n}{m!n!(\nu_{12345}-4-\varepsilon)_{n+m}(\nu_{345}-2-\varepsilon/2)_m(\nu_{345}-2-\varepsilon/2)_n},$$

which derives from a Appell–function of the first kind, F_1 .

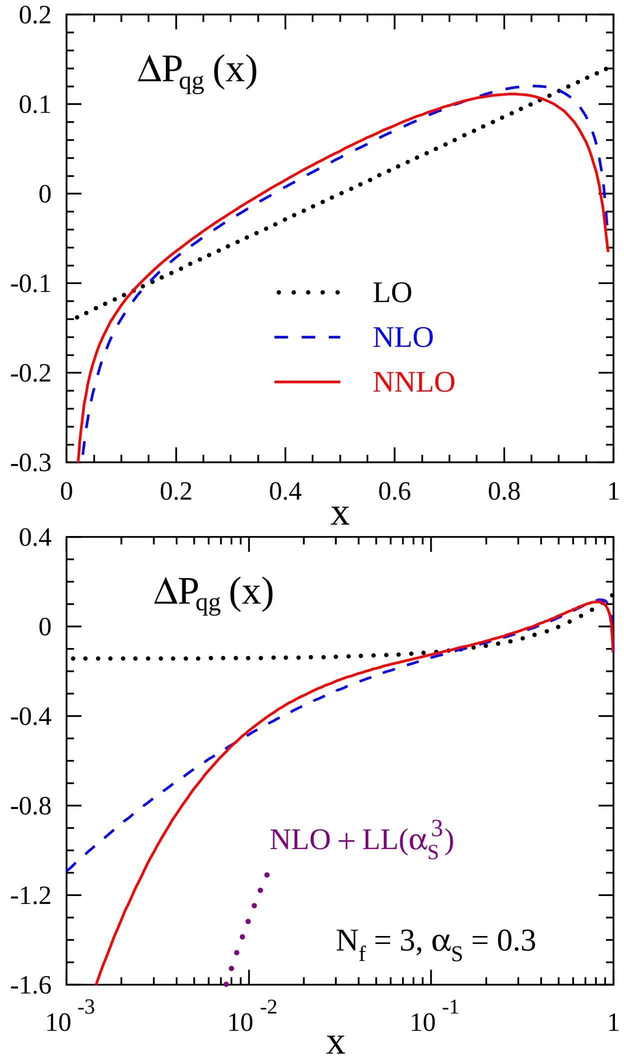
First General N Results at 3–Loop

Insert the quark-operator in the middle line :

$$L_3 = -\frac{4(N+1)S_1+4}{(N+1)^2(N+2)}\zeta_3 + \frac{2S_{2,1,1}}{(N+2)(N+3)} + \frac{1}{(N+1)(N+2)(N+3)}\Biggl\{-2(3N+5)S_{3,1} - \frac{{S_1}^4}{4}$$
$$+\frac{4(N+1)S_1-4N}{N+1}S_{2,1} + 2\Bigl((2N+3)S_1 + \frac{5N+6}{N+1}\Bigr)S_3 + \frac{9+4N}{4}{S_2}^2 + \Bigl(-\frac{5}{2}{S_1}^2 + \frac{5N}{N+1}S_1 + \frac{N}{N+1}{S_1}^3$$
$$+2\frac{7N+11}{(N+1)(N+2)}\Bigr)S_2 + \frac{2(3N+5){S_1}^2}{(N+1)(N+2)} + \frac{4(2N+3)S_1}{(N+1)^2(N+2)} - \frac{(2N+3)S_4}{2} + 8\frac{2N+3}{(N+1)^3(N+2)}\Biggr\} .$$

2. Polarized 3-loop Anomalous Dimensions

Moch,Rogal,Vermaseren,Vogt, 2008



- $\Delta P_{qq}^{NS+}(x) = P_{qq}^{NS+}(x)$
- Numerical representaion for $\Delta P_{qg}(x)$
- Other matrix entries in preparation

3. General Unfolding of Moments

Blümlein, Kauers, Klein, Schneider, 2008.

- Single scale quantities may often be more easily calculated in terms of Mellin moments
- Are there general formalisms to unfold exact formula for all N ?

$\Longrightarrow$ The corresponding quantities are recurrent in Mellin space.

- Example: Harmonic Sums or linear combinations thereof:

$$F(N+1) - F(N) = \frac{\text{sign}(a)^{N+1}}{(N+1)^{|a|}}$$

is solved by $S_a(N)$; and similarly for deeper nested sums.

- Very likely single scale Feynman diagrams do always obey difference equations.

- Assume: a finite, sufficiently large number of moments is available for a certain quantity.

- Can one determine the desired relation for general values of N free of further assumptions ?

3. General Unfolding of Moments

Method :[completely automatic]

- Apply a general recursion finder to the sequence of moments; optimize the recurrence - i.e. find low order.
- Solve the recurrence in Π and Σ fields over a basis of certain functions.
- For a while these functions are harmonic sums. At higher orders more general structures are emerging.

Examples : anomalous dimensions and massless Wilson coefficients up to 3-loop order.

- analyze by color factor.

-The recursion finder terminates its search having found one or more recursions after having tested the environment further.

-Initial values come from the given moments.

-Most demanding case: 4 weeks CPU-time, $\leq$ 10 GB

3. General Unfolding of Moments

$C_{2,q} \propto C_F^3$:

• 5114 moments needed. Use a clever way to calculate the input.

• Largest moment: fraction: numerator 13388 digits; denominator 13381 digits.

• CPU time to determine the recurrence: 20.7 days.

- modular prediction of the dimension: 4 h; modular LEQ's: 5.8 days; modular operator GCDs: 11 days; Chinese Remainder + Rat. Reconstruction: 3.8 days. 140 large primes needed.

94 MB recurrence is established; largest integer: 1227 digits; order: 35; degree: 938

• Solved by `sigma` within about one week.

• 3 loop anomalous dimensions: much smaller recurrences & shorter computation times.

$\Longrightarrow$ In practice no method does yet exists to calculate such a high number of moments.

$\Longrightarrow$ Existence proof of a quite general and powerful automatic difference-equation solver, standing rather demanding tests.