Improve Numerical Stabilities of Amplitudes in Precise QCD Calculations

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Motivation of Precise QCD Calculations

- Precise QCD calculations involves:
  - PDF sets calculated and fitted with higher order splitting function.
  - Fixed order pQCD calculations including more loops and/or legs.
  - Parton shower, resummation etc.

- Motivations:
  - Reduced theoretical uncertainty
  - Large contributions from higher order terms in pQCD
  - Better understanding of S/B in LHC
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  - Distinguish SM signal from potential new physics
- Example of cutting edge studies:
  - $pp \to H$ @ N^3LO Anastasiou et al
  - Di-jet production @ $NNLO$ Currie et al
  - top pair production @ $NNLO$ Abelof et al; Baernreuther et al
  - H+jet @ $NNLO$ Chen et al; Boughezal et al
  - Z+jet @ $NNLO$ Morgan et al
  - W+jet @ $NNLO$ Boughezal et al
  - Higgs and Drell-Yan production@ $NNLO + PS$ Hamilton et al
  - Colourless particles production@ $NNLO + NNLL$ Wiesemann et al
  - And many more $\cdots$

Matrix elements involved in fixed order pQCD

- Renormalised factorized parton level differential cross section ($d\hat{\sigma}$) for example:

$$
\begin{aligned}
d\hat{\sigma}_{LO} &= \int [\langle \mathcal{M}^0 | \mathcal{M}^0 \rangle]_{n+2} d\Phi_n J_n^{(n)} \\
d\hat{\sigma}_{NLO} &= \int [\langle \mathcal{M}^0 | \mathcal{M}^0 \rangle]_{n+3} d\Phi_{n+1} J_n^{(n+1)} \\
&+ \int [\langle \mathcal{M}^0 | \mathcal{M}^1 \rangle + \langle \mathcal{M}^1 | \mathcal{M}^0 \rangle]_{n+2} d\Phi_n J_n^{(n)} \\
d\hat{\sigma}_{NNLO} &= \int [\langle \mathcal{M}^0 | \mathcal{M}^0 \rangle]_{n+4} d\Phi_{n+2} J_n^{(n+2)} \\
&+ \int [\langle \mathcal{M}^0 | \mathcal{M}^1 \rangle + \langle \mathcal{M}^1 | \mathcal{M}^0 \rangle]_{n+3} d\Phi_{n+1} J_n^{(n+1)} \\
&+ \int [\langle \mathcal{M}^1 | \mathcal{M}^1 \rangle + \langle \mathcal{M}^2 | \mathcal{M}^0 \rangle + \langle \mathcal{M}^0 | \mathcal{M}^2 \rangle]_{n+2} d\Phi_n J_n^{(n)}
\end{aligned}
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- Higher order contributions contains both explicit (Pole structure) and implicit IR divergences (singular in unresolved P.S.).
- Whether those matrix elements are stable in unresolved P.S. is an open question.

Factorisation of implicit IR divergence (NNLO)

- Implicit IR divergent behaviour of qQCD matrix elements can be factorised.
- Colour ordered amplitudes constrain the IR divergence only in colour connected partons Mangano, Parke, Giele, Xu, Berends (1980s)
- For single unresolved limits (tree level): Define $|M^0|^2 \equiv \langle \mathcal{M}^0 | \mathcal{M}^0 \rangle$

$$|M^0(\cdots, i, j_g, k, \cdots)|^2 \xrightarrow{p_j \to 0 \sim \Delta^2} S_{ijk} |M^0(\cdots, i, k, \cdots)|^2 \sim \mathcal{O}(\Delta^{-4})$$

$$|M^0(\cdots, i, j, \cdots)|^2 \xrightarrow{p_i // p_j} \frac{1}{s_{ij}} P_{ij \to K}(z) |M^0(\cdots, K, \cdots)|^2 \sim \mathcal{O}(\Delta^{-2})$$

where $s_{ij} = (p_i + p_j)^2$, $z = p_j/(p_j + p_i)$

$$S_{ijk} = \frac{2 s_{ik}}{s_{ij} s_{jk}},$$

$$P_{qg \to Q} = P_{\bar{q}g \to \bar{Q}} = \frac{1 + (1-z)^2 - \epsilon z^2}{z},$$

$$P_{q\bar{q} \to G} = P_{\bar{q}q \to G} = \frac{z^2 + (1-z)^2 - \epsilon}{1 - \epsilon},$$

$$P_{gg \to G} = 2\left(\frac{z}{1-z} + \frac{1-z}{z} + z(1-z)\right).$$

Factorisation of implicit IR divergence (NNLO)

- For single unresolved limits (loop level): Define $|M^1|^2 \equiv \langle \mathcal{M}^0 | \mathcal{M}^1 \rangle + \langle \mathcal{M}^1 | \mathcal{M}^0 \rangle$

$$|M^1(\cdots,i,j_g,k,\cdots)|^2 \xrightarrow{p_j\ soft} S_{ijk}|M^1(\cdots,i,k,\cdots)|^2 + S^1_{ijk}|M^0(\cdots,i,k,\cdots)|^2 \sim \mathcal{O}(\Delta^{-4})$$

$$|M^1(\cdots,i,j,\cdots)|^2 \xrightarrow{p_i//p_j} \frac{1}{s_{ij}} P_{ij\to K}(z)|M^1(\cdots,K,\cdots)|^2 + \frac{1}{s_{ij}} P^1_{ij\to K}(z)|M^0(\cdots,K,\cdots)|^2 \sim \mathcal{O}(\Delta^{-2})$$

- For double unresolved limits (tree level):

$$|M^0(\cdots,a,i,j,b,\cdots)|^2 \xrightarrow{p_i,p_j\ soft} S_{aijb}|M^0(\cdots,a,b,\cdots)|^2 \sim \mathcal{O}(\Delta^{-8})$$

$$|M^0(\cdots,i,j,k,\cdots)|^2 \xrightarrow{p_i//p_j//p_k} P_{ijk\to A}(z_{1,2,3})|M^0(\cdots,A,\cdots)|^2 \sim \mathcal{O}(\Delta^{-6})$$

$$|M^0(\cdots,a,i,j,k,\cdots)|^2 \xrightarrow{p_i\ soft,\ p_j//p_k} S_{a,ijk}\frac{1}{s_{jk}} P_{jk\to K}(z)|M^0(\cdots,a,K,\cdots)|^2$$

Testing numerical stability of matrix elements

- Numerical instability comes from internal cancellation of terms with divergent order higher than the factorisation functions.
- Analytically check in each unresolved limits with known factorisation functions
  - Keep tracking of the order of divergences and find large cancellation behaviour
  - Only easy to check with small number of legs
  - Matrix elements calculated using different methods needs independent test

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- Numerically check with known factorisation functions in unresolved P.S. point
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  - Hard to relate parameters in exactly limit with unresolved P.S. points
  - Can also use special functions that converge to different factorisation functions
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  - Hard to construct by hand
- Solution is to combine analytical and numerical methods
  - Analytically check matrix elements against factorisation functions
  - Use analytical checked matrix elements to construct special functions for numerical check (Antenna functions)
  - Recycle $|M^0_{n+4}(\cdots, i, j, k, l \cdots)|^2 \to X^0_4(i, j, k, l)|M^0_{n+2}(\cdots, I, L, \cdots)|^2$

Antenna functions: multi-purpose factorisation functions

Gehrmann-De Ridder, Gehrmann, Glover

- Antenna functions constructed from normalised matrix elements
- Each function has two specified hard radiators + 1 or 2 unresolved patrons

$$X_3^0(i,j,k) \sim \frac{|M_{ijk}^0|^2}{|M_{IL}^0|^2}$$

$$X_3^1(i,j,k) \sim \frac{|M_{ijk}^1|^2}{|M_{IK}^0|^2} - X_{ijk}^0 \frac{|M_{IK}^1|^2}{|M_{IK}^0|^2}$$

$$X_4^0(i,j,k,l) \sim \frac{|M_{ijkl}^0|^2}{|M_{IL}^0|^2}$$

- One antenna function mimics multiple double or single unresolved behaviour.
- Antenna functions calculated from different ME for all parton combinations:

$$\gamma^* \to q\bar{q} \ + partons \qquad \widetilde{\mathcal{X}} \to \tilde{g} \ + partons \qquad H \to \ partons$$

- Momentum mappings give the P.S. for reduced ME:
  $3 \to 2$ or $4 \to 2$ mapping $\otimes \{FF, IF, II\}$ combinations of hard radiators.

Testing numerical stability of matrix elements

- Construct antenna subtraction terms (ATS) to mimic unresolved limits of ME
  - $ME^0 = |M^0(\cdots, i, j, k, \cdots)|^2$, $ATS^0 = X_3^0(i,j,k)|M^0(\cdots, I, K, \cdots)|^2$
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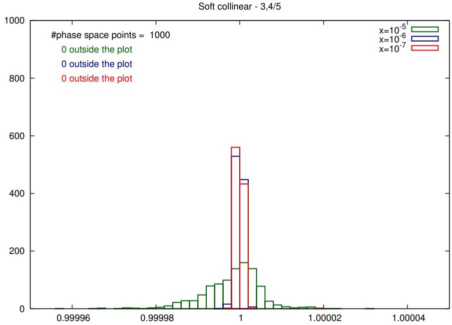
  - $ME^1 = |M^1(\cdots, i, j, k, \cdots)|^2$,
    $ATS^1 = X_3^0(i,j,k)|M^1(\cdots, I, K, \cdots)|^2 + X_3^1(i,j,k)|M^0(\cdots, I, K, \cdots)|^2$

- Test structure

$$R = \frac{ME^{0,1}}{AST^{0,1}}$$

- R ~horizontal axis (centre at one near the unresolved region)
- Number of P.S. points in each bin ~ vertical axis
- Controlling singular region correctly will achieve spike plot. For example:



$$x = \frac{s_{45}}{s}, \qquad xs = \sum_{i \neq 3} s_{3i}$$

Testing numerical stability of matrix elements

- Numerical stabilities are tested for the following ME for NNLO studies:
  - Tree level: $\mathcal{M}^0_\gamma(5P), \mathcal{M}^0(6P),\ \mathcal{M}^0_H(5P)\ (EFT),\ \mathcal{M}^0_Z(5P),\ \mathcal{M}^0_W(5P)$
  - Loop level: $\mathcal{M}^1_\gamma(4P), \mathcal{M}^1(5P),\ \mathcal{M}^1_H(4P)\ (EFT),\ \mathcal{M}^1_Z(4P),\ \mathcal{M}^1_W(4P)$
  - Generate unresolved P.S. points and test all possible limits

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  - Loop level: $\mathcal{M}^1_\gamma(4P), \mathcal{M}^1(5P),\ \mathcal{M}^1_H(4P)\ (EFT),\ \mathcal{M}^1_Z(4P),\ \mathcal{M}^1_W(4P)$
  - Generate unresolved P.S. points and test all possible limits
- Abnormal spike plots are found for single soft limits in $\mathcal{M}^1_H(4P)$ (EFT):

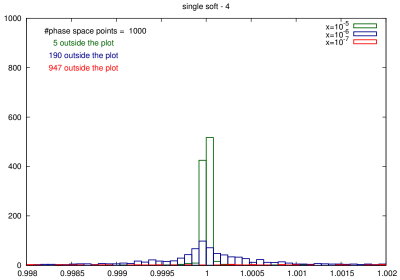

Figure: $|M^1_H(gggg)|^2$ $\quad xs = \sum_{i\neq 4} s_{4i}$

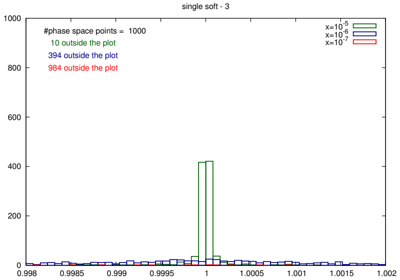

Figure: $|M^1_H(qgg\bar{q})|^2$ $\quad xs = \sum_{i\neq 3} s_{3i}$

- Identify the unstable part of the amplitude (find NAN; change precision of variable; find identical large vlaues)

Amplitudes for $\mathcal{M}_H^1(4P)$

- $\mathcal{M}_H^1(4P)$ (EFT) are calculated in hep-ph:0909.4457 and implemented in MCFM:
  - Use generalised unitarity method to construct the cut-constructible contributions.
  - A hybrid of Feynman diagram and recursive based techniques to determine the rational piece.
  - All partons are considered massless and the Higgs boson only couples to g (EFT).
- The general structure is:

$$\mathcal{M}_H^1(4P) = C_4(4P) + R_4(4P)$$

$$C_4(4P) = \sum_i C_{4;i}\mathcal{I}_{4;i} + \sum_i C_{3;i}\mathcal{I}_{3;i} + \sum_i C_{2;i}\mathcal{I}_{2;i}$$

  - $\mathcal{I}_{j;i}$ represents a j-point scalar basis integral (box, triangle, bubble)
  - $C_{j;i}$ coefficients of basis integrals are calculated by on shell tree amplitudes

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  - $\mathcal{I}_{j;i}$ represents a j-point scalar basis integral (box, triangle, bubble)
  - $C_{j;i}$ coefficients of basis integrals are calculated by on shell tree amplitudes
- Numerical instabilities in $\mathcal{M}_H^1(4P)$ come from NMHV amplitude $\mathcal{M}_H^1(1^+, 2^-, 3^-, 4^-)$:
  - $C_{3;1234|12|34}$ coefficient of three mass triangle integral
  - Large cancellation of terms between $C_4(4P)$ and $R_4(4P)$

Rewrite three-mass coefficients for $\mathcal{M}_H^1(4P)$

- The finite contributions of cut-constructible contributions contain:

$$C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-) \sim C_{3;1234|12|34}(H, 1_g^+, 2_g^-, 3_g^-, 4_g^-)\mathcal{I}_{3,3m}(m_H^2, s_{12}, s_{34})$$

with $(s_{ij} = \langle ij\rangle [ji])$

$$C_{3;1234|12|34}(H, 1_g^+, 2_g^-, 3_g^-, 4_g^-) = \sum_{\gamma=\gamma_\pm} \frac{m_H^4 \langle 34\rangle^3 \langle 2|K_1^\flat|1] \langle 2|K_1^\flat|3] \langle 2|K_1^\flat|4]}{2\gamma(\gamma + m_H^2)\langle 12\rangle s_{1K_1^\flat} s_{3K_1^\flat} s_{4K_1^\flat}}$$

$$K_1^{\flat\mu} = \gamma \frac{\gamma K_1^\mu - K_1^2 K_2^\mu}{\gamma^2 - K_1^2 K_2^2}$$

where K_1, K_2 (and K_3) are the momenta of the three off-shell legs and where γ is determined by the two solutions that ensure that $K_1^\flat$ is light-like

$$K_1^\mu = -p_1^\mu - p_2^\mu - p_3^\mu - p_4^\mu, \qquad K_2^\mu = p_1^\mu + p_2^\mu, \qquad K_3^\mu = p_3^\mu + p_4^\mu$$

$$\gamma^2 - 2K_1 \cdot K_2 \gamma + K_1^2 K_2^2 = 0$$

$$\gamma_\pm = K_1 \cdot K_2 \pm \sqrt{(K_1 \cdot K_2)^2 - K_1^2 K_2^2}$$

Rewrite three-mass coefficients for $\mathcal{M}_H^1(4P)$

- Solutions of γ satisfy following identities:

$$\gamma_+ + \gamma_- = 2K_1 \cdot K_2, \qquad \gamma_+\gamma_- = K_1^2 K_2^2,$$
$$(\gamma_- + K_1^2)(\gamma_+ + K_1^2) = K_1^2 K_3^2,$$
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- In general $C_{3;K_1|K_2|K_3}$ is sensitive to the three massive momentum inputs K_1, K_2 and K_3 when one of the legs becomes massless (e.g. $K_3^2 \to 0$):

$$-2K_1 \cdot K_2 \to K_1^2 + K_2^2 \qquad \gamma_+ \to -K_2^2 \qquad \gamma_- \to -K_1^2$$

- A potentially large cancellation for example is inside $s_{3K_1^\flat}$:

$$s^-_{3K_1^\flat} = \frac{-\gamma_-(K_1^2 + \gamma_-)(s_{13} + s_{23}) - \gamma_-^2 s_{34}}{\gamma_-^2 - K_1^2 K_2^2},$$

- The result of $(K_1^2 + \gamma_-)$ in $K_3^2 \to 0$ limit is analytically proportional to the small value $K_3^2 = s_{34}$.
- Numerically unstable when the result of large cancellation is combined with small values.

Rewrite three-mass coefficients for $\mathcal{M}_H^1(4P)$

- Rewrite $s^-_{3K_1^\flat}$ using identities of $\gamma_\pm$:

$$s^-_{3K_1^\flat} = -\frac{\gamma_- s_{34} m_H^2}{\gamma_+(\gamma_-^2 - m_H^2 s_{12})(m_H^2 + \gamma_+)}\left(\frac{m_H^2 s_{12} s_{34}}{\gamma_- + s_{12}} - (s_{14} + s_{24} + s_{34})\gamma_+\right)$$

- $s^-_{3K_1^\flat}$ is explicitly proportional to the s_{34} and there are no large cancellations
- $s^-_{4K_1^\flat}$ in $C_{3;1234|12|34}(H, 1_g^+, 2_g^-, 3_g^-, 4_g^-)$ has similar issue
- $C_{3;1234|12|34}(H, 1_{\bar{q}}^-, 2_q^+, 3_g^-, 4_g^-)$ and $C_{3;1234|41|23}(H, 1_{\bar{q}}^-, 2_q^+, 3_g^-, 4_g^-)$

Rewrite cut-completion terms for $\mathcal{M}_H^1(4P)$

- Counting the order of divergence (Δ^{-1}) in single soft limit ($p_2 \to 0 \sim \Delta^2$):

$$\langle 2i\rangle, [2i] \sim \Delta, \qquad s_{i2} \sim \Delta^2$$

- The overall divergence of the $\mathcal{M}_H^1(4P)$ amplitude should be $\mathcal{O}(\Delta^{-2})$, however there are terms of $\mathcal{O}(\Delta^{-4})$ inside $\mathcal{M}_H^1(4P)$:

$$\begin{aligned} C_4(1_g^+,2_g^-,3_g^-,4_g^-) \sim & \\ & + \frac{\langle 34\rangle[41]\left(3s_{124}\langle 34\rangle[41] + \langle 24\rangle\langle 3|p_H|1][42]\right)}{3[42]^2}\hat{L}_2\left(s_{124},s_{12}\right) \\ & + \left(\frac{2s_{124}\langle 34\rangle^2[41]^2}{\langle 24\rangle[42]^3} - \frac{\langle 24\rangle\langle 3|p_H|1]^2}{3s_{124}[42]}\right)\hat{L}_1\left(s_{124},s_{12}\right) \\ & + \frac{\langle 3|p_H|1](4s_{124}\langle 34\rangle[41] + \langle 3|p_H|1](2s_{14}+s_{24}))}{s_{124}\langle 24\rangle[42]^3}\hat{L}_0\left(s_{124},s_{12}\right) \end{aligned}$$

$$R_4(1_g^+,2_g^-,3_g^-,4_g^-) \sim \frac{[14]^2\langle 43\rangle^2}{2s_{12}[42]^2}$$

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- The cut-completion terms are defined as

$$
\begin{aligned}
\hat{L}_3(s,t) &= L_3(s,t) - \frac{1}{2(s-t)^2}\left(\frac{1}{s}+\frac{1}{t}\right), \\
\hat{L}_2(s,t) &= L_2(s,t) - \frac{1}{2(s-t)}\left(\frac{1}{s}+\frac{1}{t}\right), \\
\hat{L}_1(s,t) &= L_1(s,t), \qquad \hat{L}_0(s,t) = L_0(s,t), \qquad L_k(s,t) = \frac{\log(s/t)}{(s-t)^k}
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\end{aligned}$$

- Identities for cut-completion terms

$$\begin{aligned}
&s\hat{L}_3(s,t) = t\hat{L}_3(s,t) + \hat{L}_2(s,t),\\
&s\hat{L}_2(s,t) = t\hat{L}_2(s,t) + \hat{L}_1(s,t) - \frac{1}{2}\left(\frac{1}{s}+\frac{1}{t}\right),\\
&\frac{1}{s}\hat{L}_1(s,t) = \hat{L}_2(s,t) - \frac{t}{s}\hat{L}_2(s,t) + \frac{1}{2s}\left(\frac{1}{s}+\frac{1}{t}\right),\\
&s\hat{L}_1(s,t) = t\hat{L}_1(s,t) + \hat{L}_0(s,t), \qquad \frac{1}{s}\hat{L}_0(s,t) = \hat{L}_1(s,t) - \frac{t}{s}\hat{L}_1(s,t)
\end{aligned}$$

Rewrite cut-completion terms for $\mathcal{M}_H^1(4P)$

- Inserting $\langle 3|p_H|1] = -\langle 32\rangle[31] - \langle 34\rangle[41]$ into $C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-)$:

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$$C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-) \sim \frac{\langle 34\rangle^2[41]^2}{3[42]^2}\Bigg(+ 3s_{124}\hat{L}_2 - \frac{3}{s_{124}}\hat{L}_0 + \frac{1}{s_{24}}(6s_{124}\hat{L}_1 - 6\hat{L}_0 - \frac{6s_{12}}{s_{124}}\hat{L}_0)\Bigg) \sim \mathcal{O}(\Delta^{-4})$$

- Repeat using identities for cut-completion terms, we can rewrite:

$$\frac{\langle 34\rangle^2[41]^2}{3[42]^2}\left(3s_{124}\hat{L}_2 - \frac{3}{s_{124}}\hat{L}_0\right) =$$

$$\frac{\langle 34\rangle^2[41]^2}{[42]^2}\left(s_{12}\hat{L}_2 + \frac{s_{12}}{s_{124}}\hat{L}_1 - \frac{1}{2}\left(\frac{1}{s_{124}} + \frac{1}{s_{12}}\right)\right) \sim \mathcal{O}(\Delta^{-2}) - \frac{\langle 34\rangle^2[41]^2}{2s_{12}[42]^2}$$

$$\frac{\langle 34\rangle^2[41]^2}{3[42]^2 s_{24}}\left(6s_{124}\hat{L}_1 - 6\hat{L}_0 - \frac{6s_{12}}{s_{124}}\hat{L}_0\right) = \frac{\langle 34\rangle^2[41]^2}{[42]^2 s_{24}}\left(\frac{2s_{12}^2}{s_{124}}\hat{L}_1\right) \sim \mathcal{O}(\Delta^0)$$

Rewrite cut-completion terms for $\mathcal{M}_H^1(4P)$

- Inserting $\langle 3|p_H|1] = -\langle 32\rangle[31] - \langle 34\rangle[41]$ into $C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-)$:

$$C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-) \sim \frac{\langle 34\rangle^2[41]^2}{3[42]^2}\Bigg(+ 3s_{124}\hat{L}_2 - \frac{3}{s_{124}}\hat{L}_0 + \frac{1}{s_{24}}(6s_{124}\hat{L}_1 - 6\hat{L}_0 - \frac{6s_{12}}{s_{124}}\hat{L}_0)\Bigg) \sim \mathcal{O}(\Delta^{-4})$$

- Repeat using identities for cut-completion terms, we can rewrite:

$$\frac{\langle 34\rangle^2[41]^2}{3[42]^2}\left(3s_{124}\hat{L}_2 - \frac{3}{s_{124}}\hat{L}_0\right) =$$

$$\frac{\langle 34\rangle^2[41]^2}{[42]^2}\left(s_{12}\hat{L}_2 + \frac{s_{12}}{s_{124}}\hat{L}_1 - \frac{1}{2}\left(\frac{1}{s_{124}} + \frac{1}{s_{12}}\right)\right) \sim \mathcal{O}(\Delta^{-2}) - \frac{\langle 34\rangle^2[41]^2}{2s_{12}[42]^2}$$

$$\frac{\langle 34\rangle^2[41]^2}{3[42]^2 s_{24}}\left(6s_{124}\hat{L}_1 - 6\hat{L}_0 - \frac{6s_{12}}{s_{124}}\hat{L}_0\right) = \frac{\langle 34\rangle^2[41]^2}{[42]^2 s_{24}}\left(\frac{2s_{12}^2}{s_{124}}\hat{L}_1\right) \sim \mathcal{O}(\Delta^0)$$

- Cancellation with $R_4(1_g^+, 2_g^-, 3_g^-, 4_g^-) \sim \frac{[14]^2\langle 43\rangle^2}{2s_{12}[42]^2}$

Improve numerical stability of matrix elements

- After rewriting of $C_4(1_g^+, 2_g^-, 3_g^-, 4_g^-)$ and $R_4(1_g^+, 2_g^-, 3_g^-, 4_g^-)$:

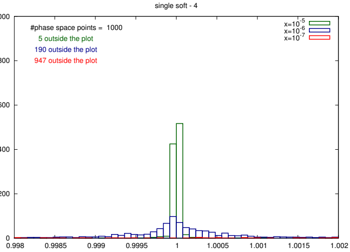

Figure: $|M_H^1(gggg)|^2$ unstable

$\rightarrow$

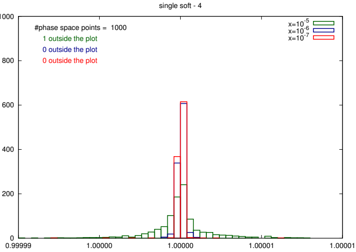

Figure: $|M_H^1(gggg)|^2$ stable

- $|M_H^1(qgg\bar{q})|^2$ and $|\hat{M}_H^1(gggg)|^2$ can achieve spike plots with the same treatment

Summary

- Precise QCD calculations require amplitudes for higher orders
- More and more efforts are required to obtain amplitudes with more loops and legs. We also need these amplitudes to be IR stable in unresolved P.S.
- Subtraction terms from phenomenology studies can be used to test the IR behaviour of amplitudes
- Examples of identifying large cancellations and rewriting amplitudes are introduced in this talk
- Testing of more amplitudes are needed

Back up slides

Improve numerical stability of matrix elements