QWG 2024 - IISER Mohali

FKS Subtraction for Quarkonium Production & Automation in MadGraph5_aMC@NLO

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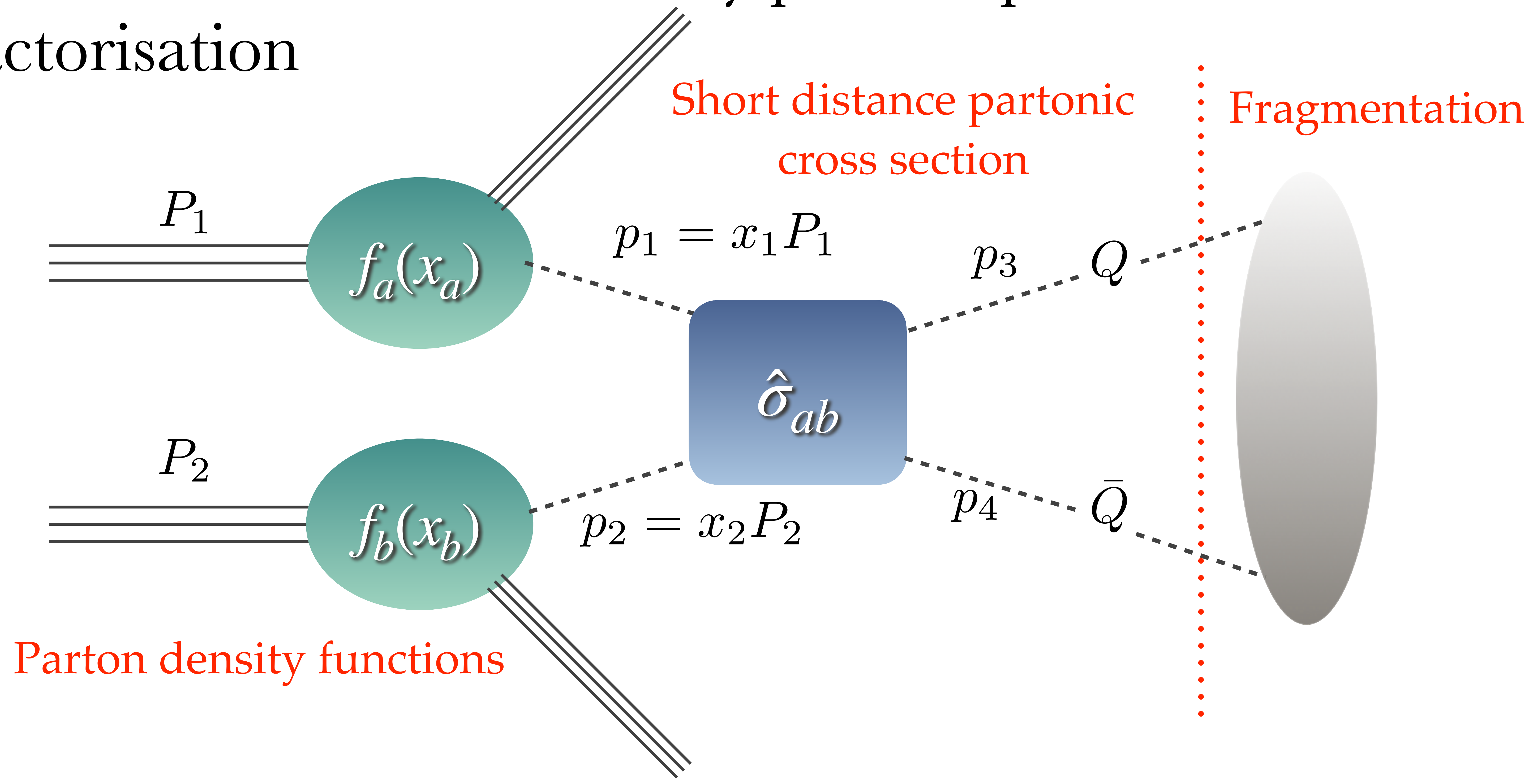
What & Why Subtraction : Motivation

- Let us start from elementary particle productions described using collinear factorisation



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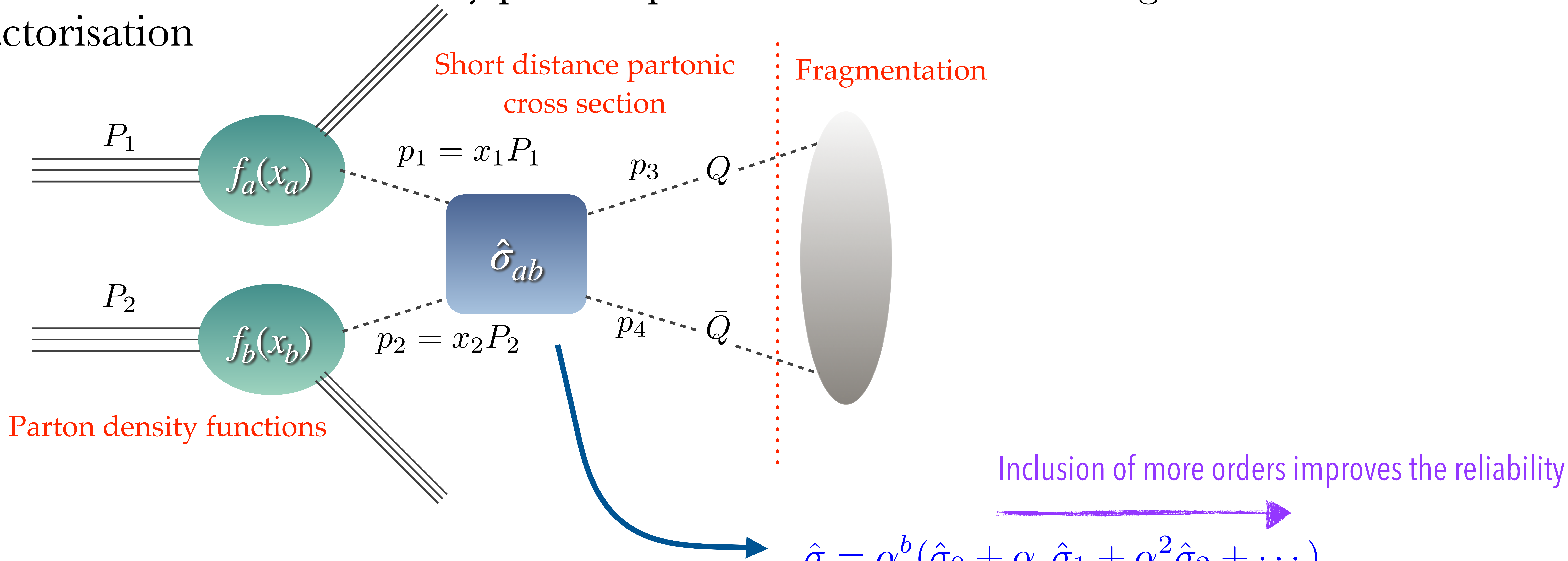

$$\hat{\sigma} = \alpha_s^b(\hat{\sigma}_0 + \alpha_s\hat{\sigma}_1 + \alpha_s^2\hat{\sigma}_2 + \cdots)$$

LO NLO NNLO

pQCD

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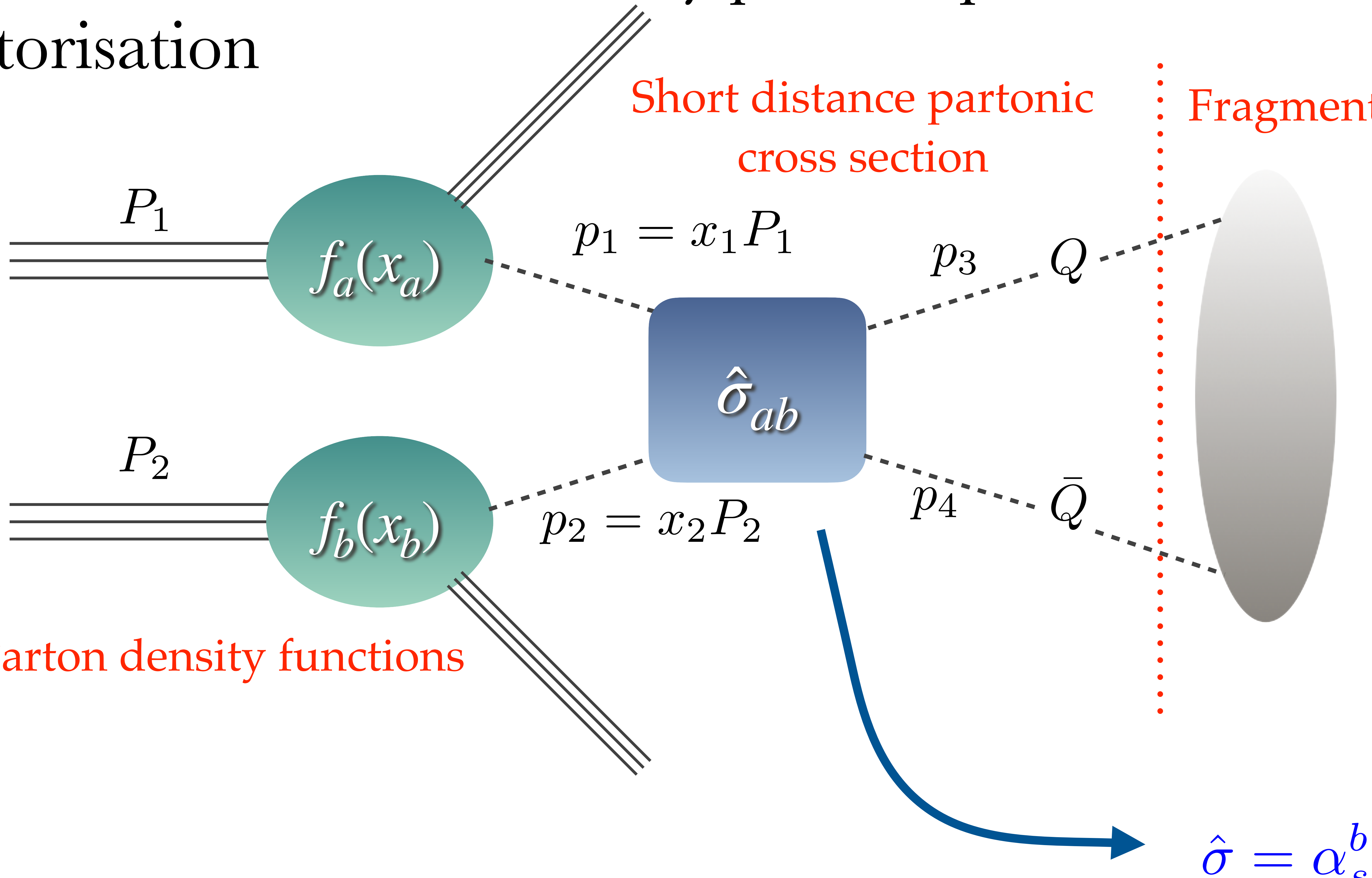


At least NLO is required for reliable study

Inclusion of more orders improves the reliability

$$\hat{\sigma} = \alpha_s^b(\hat{\sigma}_0 + \alpha_s\hat{\sigma}_1 + \alpha_s^2\hat{\sigma}_2 + \cdots)$$

LO NLO NNLO

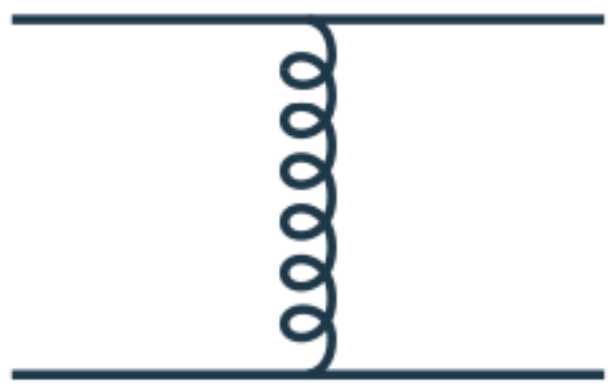
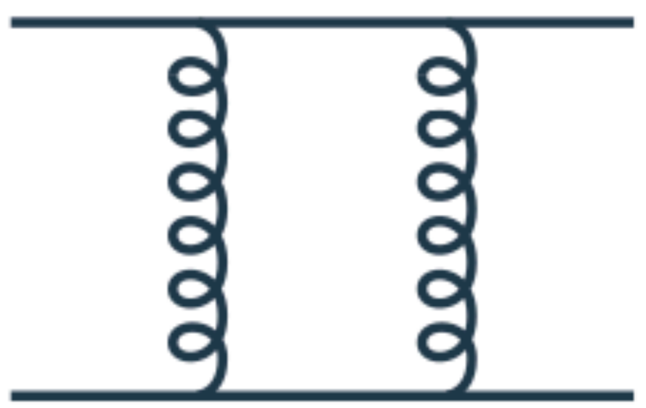
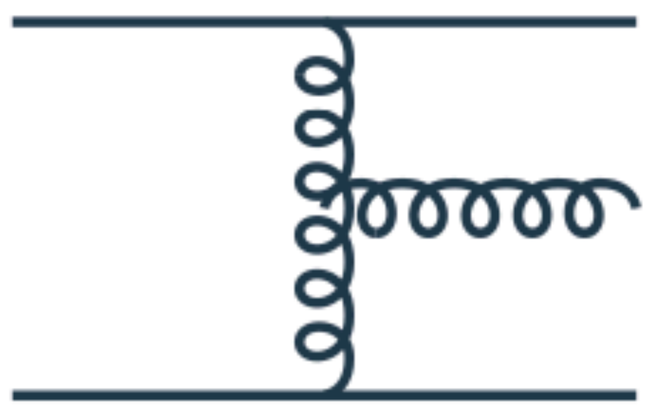
pQCD

What & Why Subtraction : NLO brief

Born cross section	Virtual corrections	Real corrections

$$\sigma_{\mathrm{NLO}} = \int d\phi_n \mathcal{B} + \int d\phi_n \mathcal{V} + \int d\phi_{n+1} \mathcal{R}$$

$\mathcal{O}(\alpha_s^b)$ $\mathcal{O}(\alpha_s^{b+1})$ $\mathcal{O}(\alpha_s^{b+1})$

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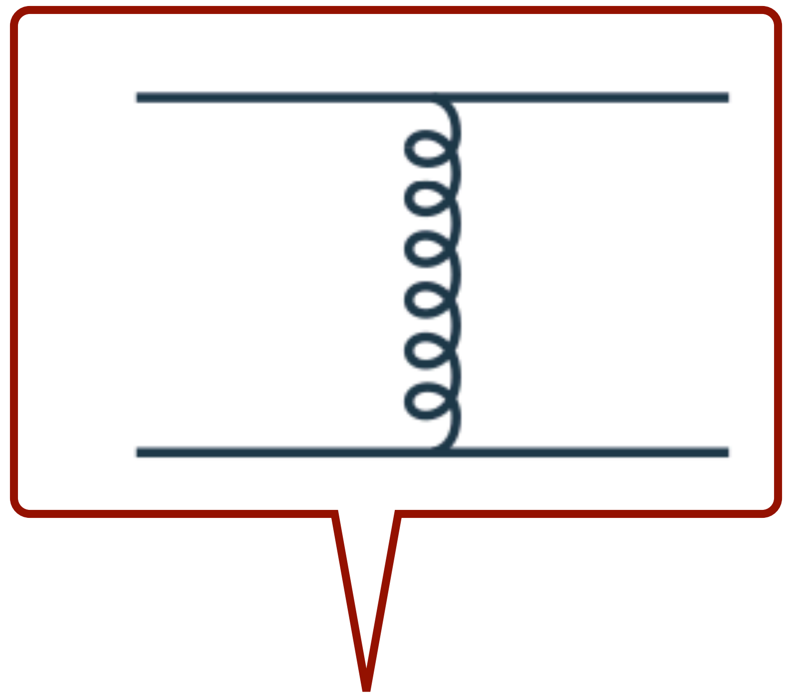
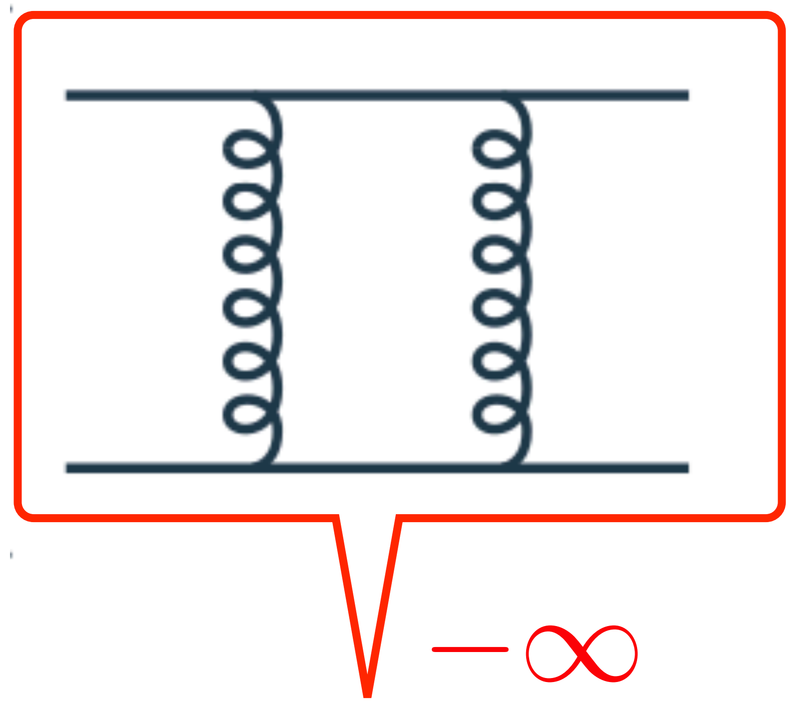
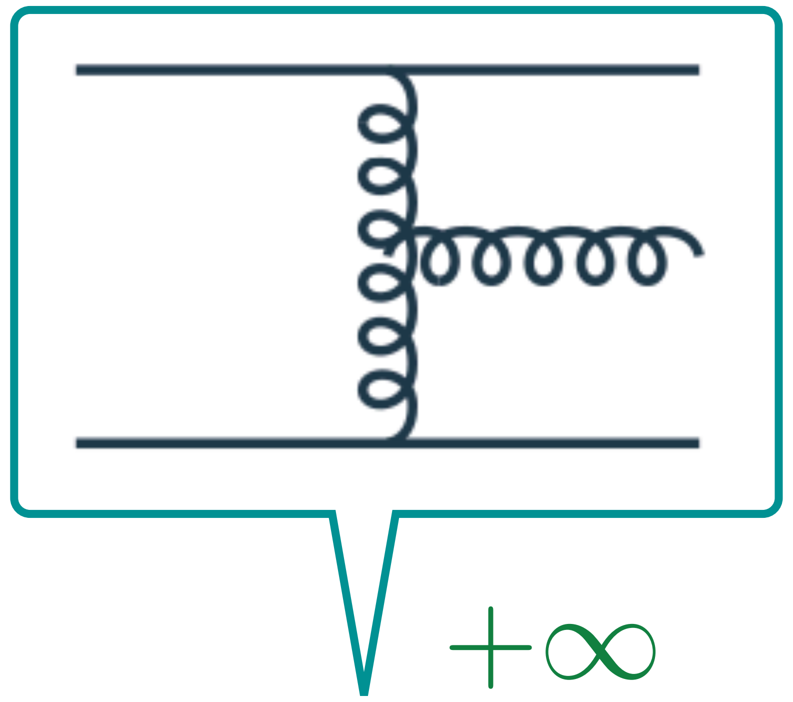




$-\infty$



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Finite

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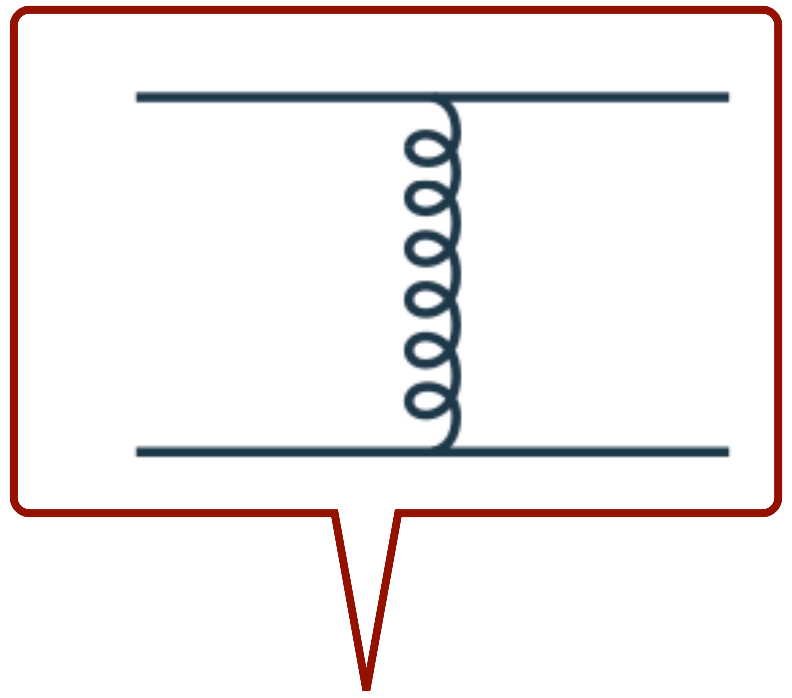

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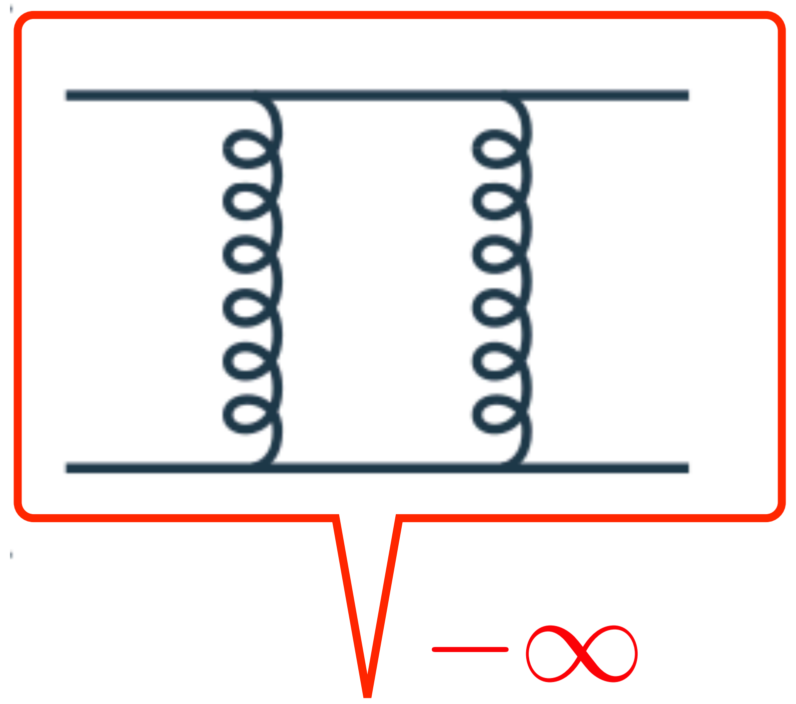
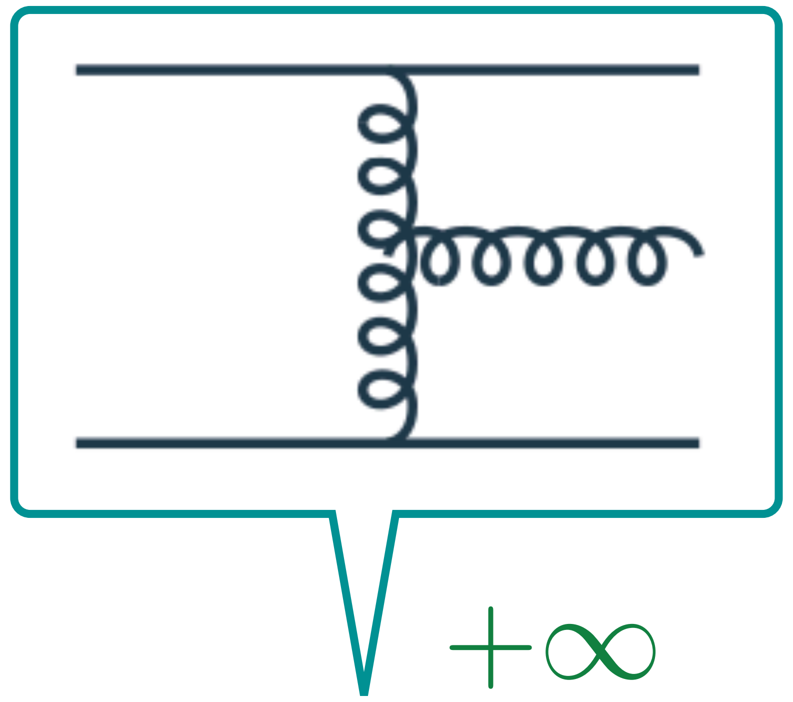


$-\infty$

$$\mathcal{V} = \frac{A}{\epsilon^2} + \frac{B}{\epsilon} + \mathcal{V}_{\text{finite}}$$



$+\infty$

$$\int d\phi_1 \mathcal{R} = -\frac{A}{\epsilon^2} - \frac{B}{\epsilon} + \mathcal{R}_{\text{finite}}$$

Cure:

Partonic cross section is infrared safe

-KLN theorem

[Kinoshita '62; Lee, Nauenberg '64]

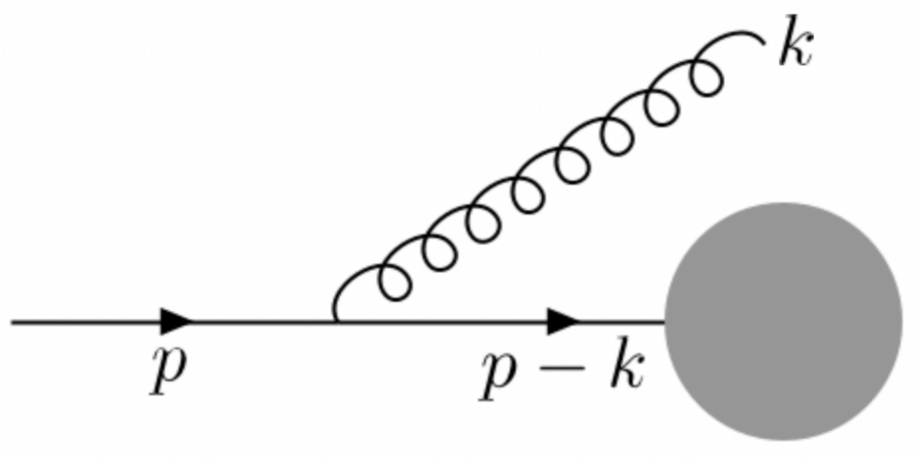
Individually divergent , however $\mathcal{V} + \int d\phi_1 \mathcal{R} = \text{infrared safe}$

What & Why Subtraction : NLO brief

- Matrix elements for the real emission has a complex structure. Hence, the phase space integration over it is really hard.
- In practice, we explore different numerical tools such as Monte-Carlo techniques to perform this phase space integration.
- But the problem is the IR divergence that appears in some corners of the phase space of radiated parton. So we need to get rid of them before we attempt the integration.
- That is exactly where the role of subtraction comes!

How subtraction Works?

- Conceptually straightforward : find out the origin of the singularities and subtract them from the real emissions.
- Let us see the source of these divergences:



$$\left| \quad \right|^2 \sim \frac{1}{k \cdot p} = \frac{1}{E_g E_q (1 - \cos\theta_{gq})}$$

$$\longrightarrow \infty \begin{cases} \text{when } E_g \to 0 & \textit{soft singularity} \\ \text{when } \theta_{gq} \to 0 & \textit{collinear singularity} \end{cases}$$

Divergence appears due to soft and/or collinear emissions

How subtraction Works?

$$\int d\phi_1 \mathcal{R} \to \underbrace{\int d\phi_1 (\mathcal{R} - \mathcal{S})} + \boxed{\int d\phi_1 \mathcal{S}}$$

$$\lim_{E_i \to 0} \mathcal{S} = \lim_{E_i \to 0} \mathcal{R}$$

$$\lim_{\theta_{ij} \to 0} \mathcal{S} = \lim_{\theta_{ij} \to 0} \mathcal{R}$$

$\mathcal{S} \to$ Subtraction counter term

Free of divergences. Numerical integration possible in 4-dim.

Integrated counter term, to be added back

Their divergence cancels with those of virtual corrections

- Requirement to choose a subtraction term:
  - Should exactly matches the real emissions in their singular limits.
  - Simple enough to integrate exactly.

NLO with subtraction

$$\sigma_{\rm NLO} = \int d\phi_n \; \mathcal{B}$$

$$+ \int d\phi_n \left(\mathcal{V} + \int d\phi_1 \mathcal{S} \right)_{\epsilon \to 0}$$

$$+ \int d\phi_{n+1} (\mathcal{R} - \mathcal{S})$$

Each of the integrand is finite and can be integrated numerically in 4-dimension and independently from one another

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- Widely used subtraction methods at NLO
  - ➡ Dipole subtraction method [Catani, Seymour '96]
  - ➡ FKS subtraction method [Frixione, Kunszt, Signer '95]

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General for any QCD process

Automated in MadGraph_aMC@NLO (MG5) [Frederix, Frixione, Maltoni, Stelzer '09]

& POWHEG BOX

[Alioli, Nason, Oleari, Re '10]

NLO Automation in MG5

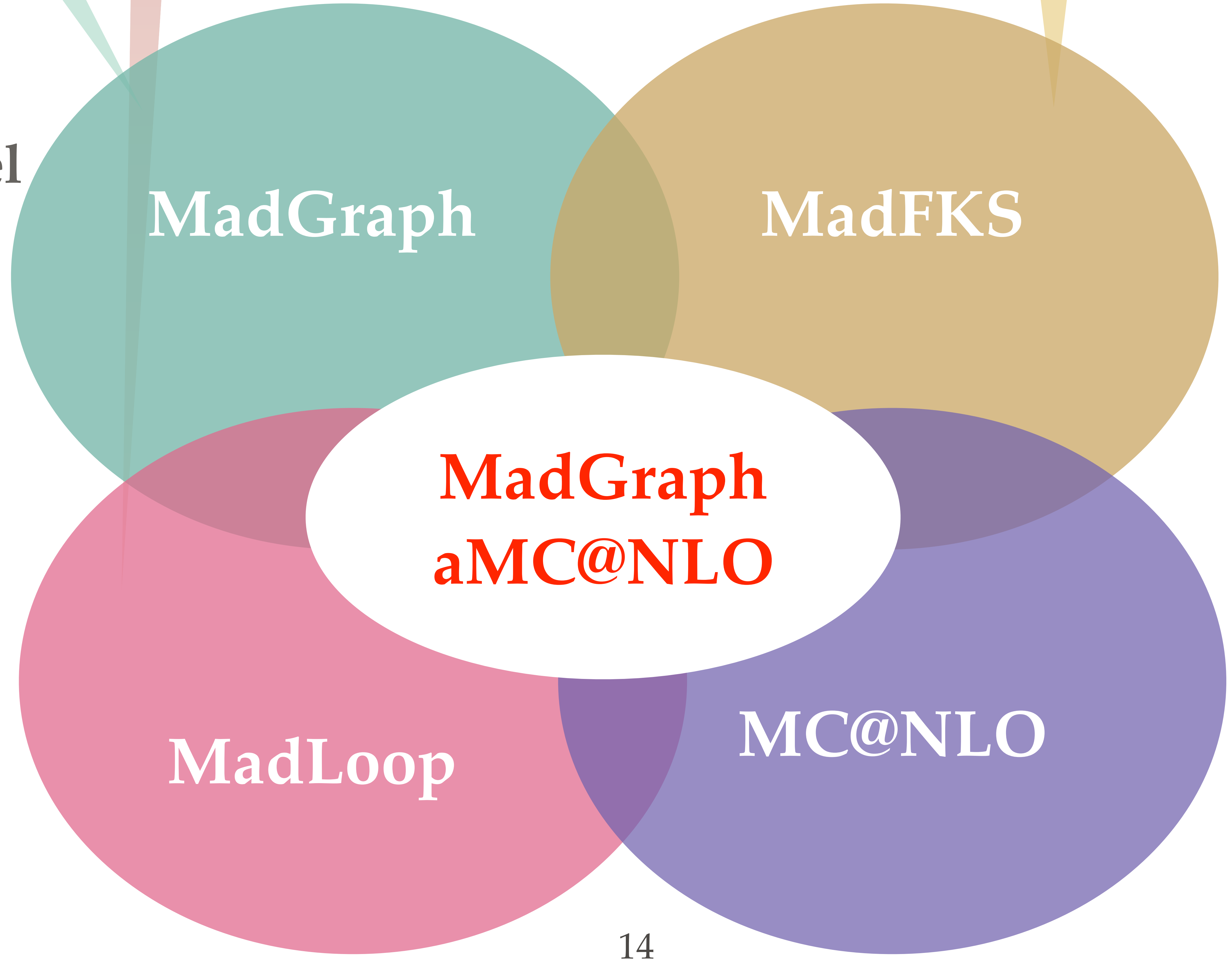
[Alwall, Frederix, Frixione, Hirschi, Maltoni, Mattelaer, Shao, Stelzer, Torrielli, Zaro '14]

$$\sigma_{\rm NLO} = \int d\phi_n \mathcal{B} + \int d\phi_n \mathcal{V} + \int d\phi_n \int d\phi_1 \mathcal{S} + \int d\phi_{n+1} \left(\mathcal{R} - \mathcal{S}\right)$$

Automatic tree level matrix element generator

SM and BSM

Automation of real correction using FKS subtraction



Automation of virtual corrections

Matching & Merging

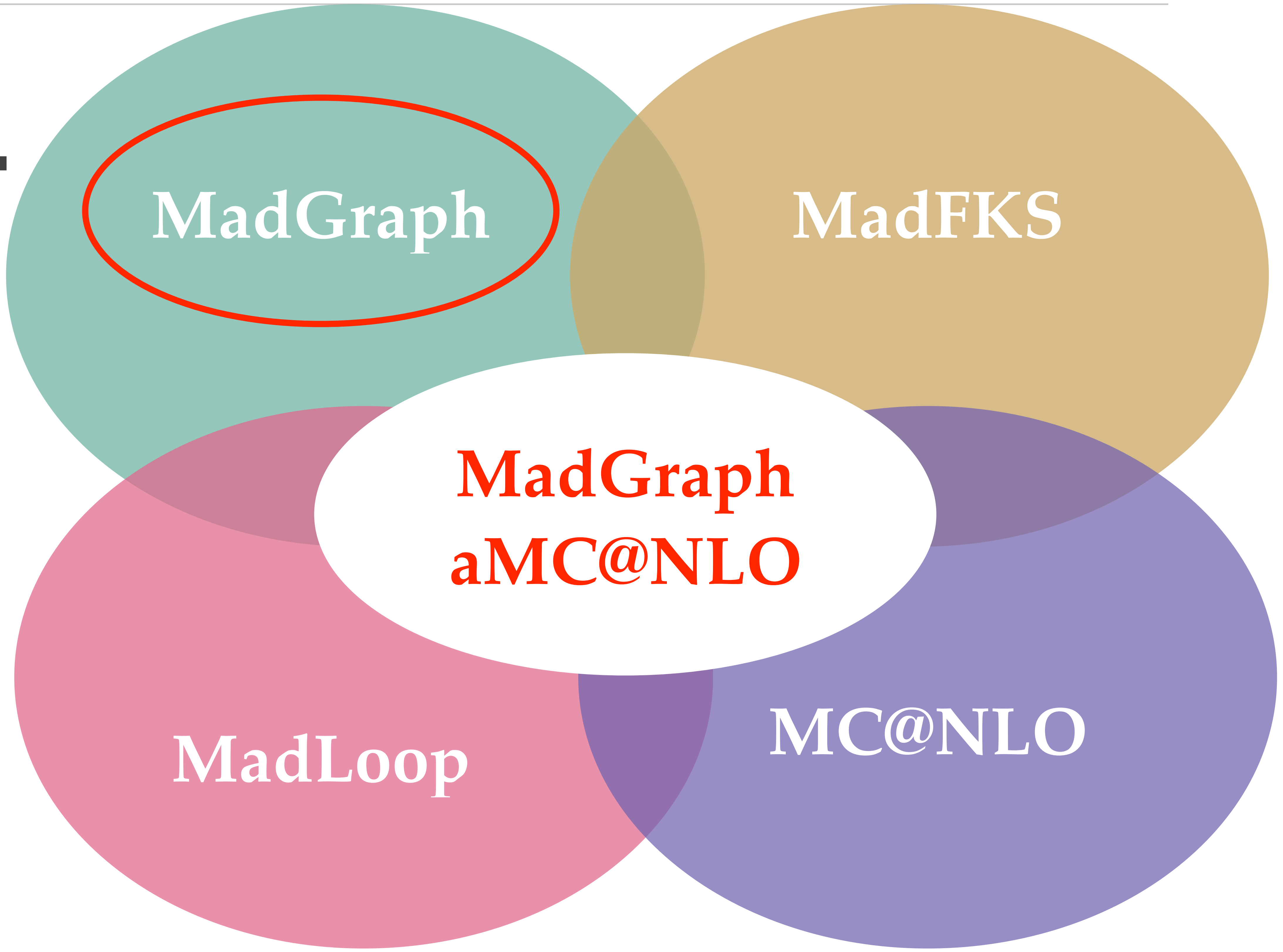
NLO Automation in MG5 - for Quarkonium

- Master formula : NRQCD factorisation

$$d\sigma(AB \to H + X) = \sum_n \Big(\sum_{a,b,X} \int dx_a dx_b f_{a/A}(x_a) f_{b/B}(x_b) \times d\hat{\sigma}(ab \to Q\bar{Q}'[n] + X) \Big) \langle \mathcal{O}_n^H \rangle$$

LDME

Short distance cross section
for heavy quark bound state with a specific color (C), spin(S) and orbital (L) and total (J) angular momentum state :
$n = {}^{2S+1}L_J^{[C]}$



- Amplitude : $\mathcal{A}_{a+b\to Q\bar{Q}'[n]} = \mathbb{P}_J \mathbb{P}_L \mathbb{P}_S \mathbb{P}_C \mathcal{A}_{a+b\to Q\bar{Q}'}$

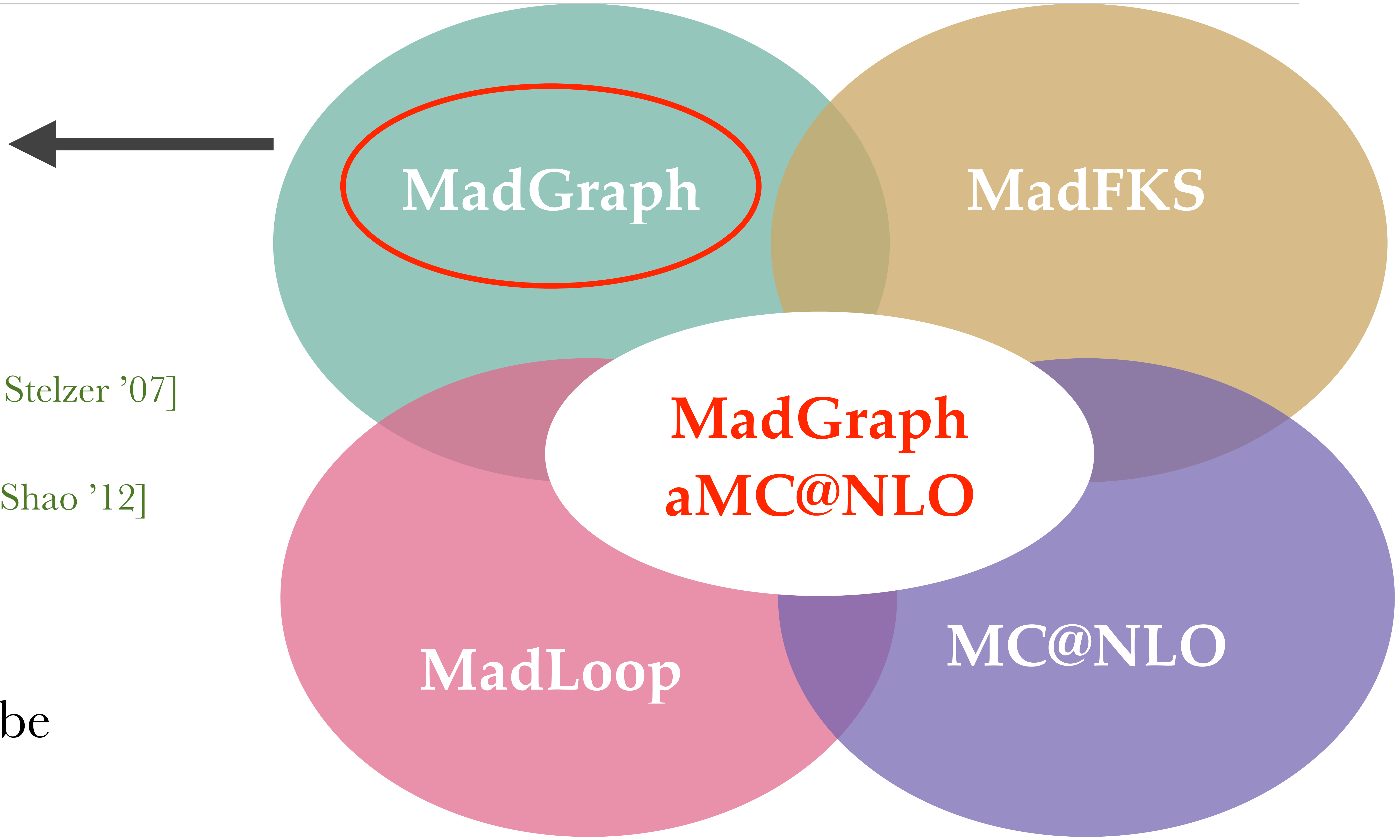
Projection operators

NLO Automation in MG5 - for Quarkonium

- For automation at tree level, already available tools in the market:

  MadOnia : for single quarkonium
  [P. Artoisenet, F. Maltoni and T. Stelzer '07]

  HELAC-Onia : general for one or more quarkonium [H.S Shao '12]



- Automating beyond tree level : best way could be extending the MG5 by including general quarkonium productions.

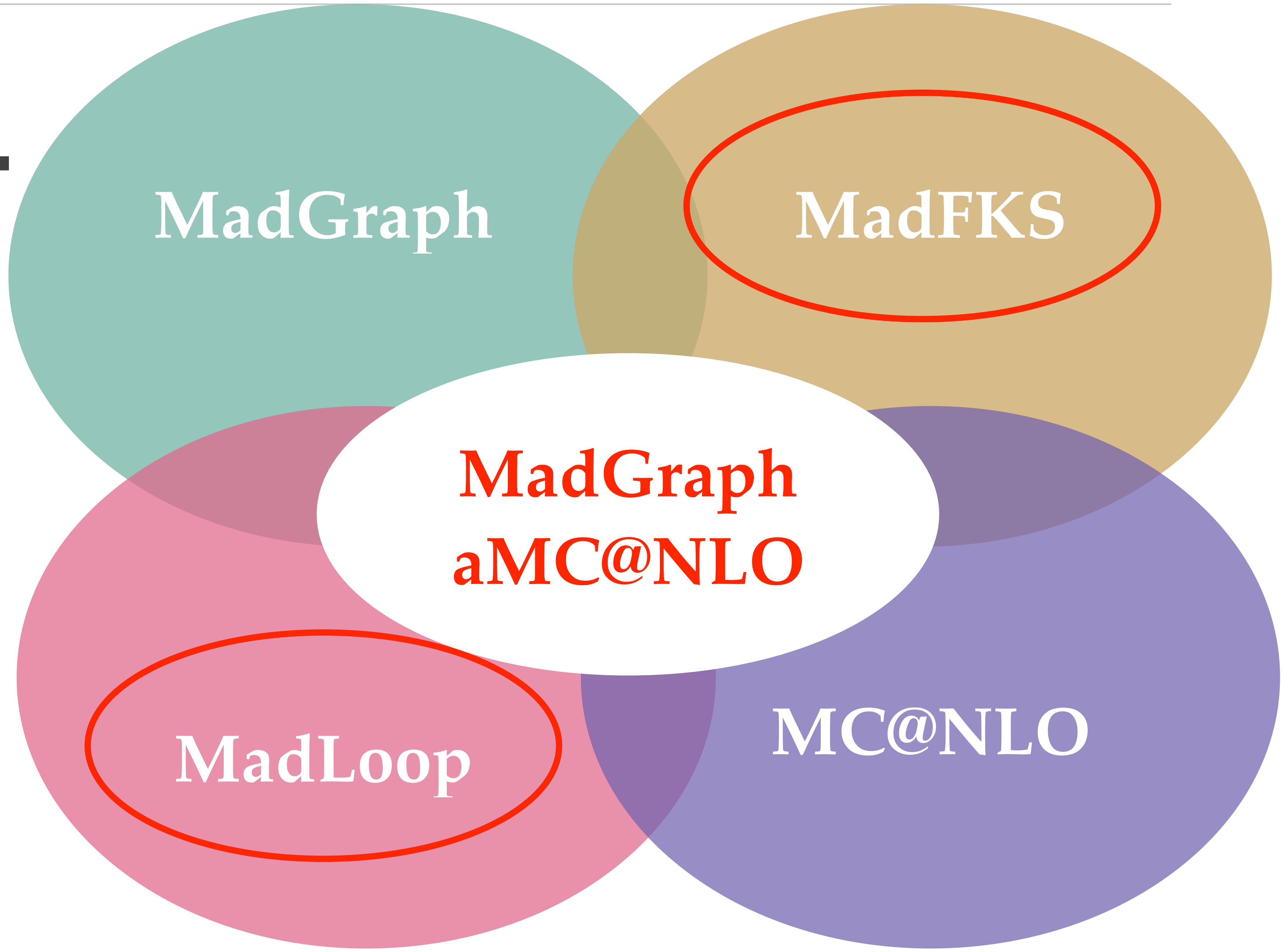
  Ongoing work - H.S Shao, Chris Flett et.al
  Implementation of projection operators required

NLO Automation in MG5 - for Quarkonium

- Automating beyond tree level : at NLO
  - Extend MadLoop : future work
  - Extend MadFKS

First step : Extend FKS subtraction method by finding out the counter terms (& integrated) required for additional divergences due to radiation from heavy quarkonia.

Aim of our work



FKS in brief

- Basic idea of FKS : partition the phase space such that each region involves only one soft and/or collinear singularities

$$\sum_{ij-pairs} S_{ij} = 1$$

$$d\sigma_{\mathcal{R}} = |\mathcal{M}_{n+1}|^2 \, d\phi_{n+1}$$

Partition function

$$= \sum_{ij-pairs} S_{ij} |\mathcal{M}_{n+1}|^2 \, d\phi_{n+1}$$

$$S_{ij} = \begin{cases} 1 \text{ if } p_i \cdot p_j \to 0 \\ 0 \text{ if } p_m \cdot p_n \to 0, \{m,n\} \neq \{i,j\} \end{cases}$$

- The subtraction term, for example for the soft emission of i^{th} gluon, can be obtained as

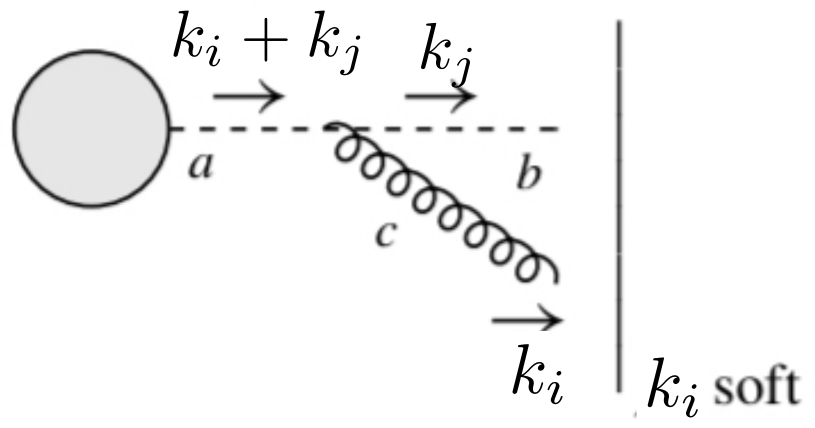
$$\mathcal{S}_{\text{soft}} = \lim_{\xi_i \to 0} \sum_j S_{ij} |\mathcal{M}_{n+1}|^2$$

- Counter terms are maximally from three regions
  - Soft
  - Collinear
  - Soft-collinear

Subtracting all of them from real corrections give finite contributions

FKS in brief

- Additionally, we have to add back integrated counter term as well $\int d\phi_1 \mathcal{S}_{\rm soft}$



- For this we have soft-eikonal approximation :

$$\lim_{k_i \to 0} \mathcal{A}^{(n+1,0)}(r) = g_s \frac{k_j \cdot \varepsilon^*_{\lambda_i}(k_i)}{k_j \cdot k_i} \vec{Q}(\mathcal{I}_j) \mathcal{A}^{(n,0)}(r^{\not{i}})$$

- At the amplitude squared level, this boil down to evaluating Eikonal integrals of the form

$$\int d\Omega_i \frac{k_k \cdot k_l}{(k_k \cdot k_i)(k_l \cdot k_i)}$$

- This is known for general massive/massless cases [Frederix, Frixione, Maltoni, Stelzer '09]

Extending FKS to quarkonium

- What is new?
  - additional singularities appear due to the radiation emitted from quarkonia states
    - Soft in origin - from projection operators and LDME renormalisation
    - No new collinear or soft-collinear divergences : because *heavy* quarkonium
  - Additional non-standard Eikonal integrals

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    We can proceed similar methods to get new local counter terms to remove new singularities

  - Additional non-standard Eikonal integrals

    Need to evaluate the non-standard integrals

Extending FKS to quarkonium

- Let us see an example of $\left({}^1P_1^{[8]}\right)$
- The amplitude after applying the projection operator gives

$$\lim_{k_i \to 0} \mathcal{A}^{(n+1,0)}_{\{[8],0,1,1\}}(r) = \sum_{\substack{j=n_I \\ j\neq i}}^{n_L^{(R)}+n_H} g_s \frac{k_j \cdot \varepsilon^*_{\lambda_i}(k_i)}{k_j \cdot k_i} \vec{Q}(\mathcal{I}_j) \mathcal{A}^{(n,0)}_{\{[8],0,1,1\}}(r^{\not{i}}) + g_s \frac{K \cdot \varepsilon^*_{\lambda_i}(k_i)}{K \cdot k_i} \vec{Q}(Q\bar{Q}'[{}^1P_1^{[8]}]) \mathcal{A}^{(n,0)}_{\{[8],0,1,1\}}(r^{\not{i}})$$

$$+ g_s \left[\frac{\varepsilon^*_{\lambda_l}(K) \cdot \varepsilon^*_{\lambda_i}(k_i)}{K \cdot k_i} - \frac{K \cdot \varepsilon^*_{\lambda_i}(k_i) k_i \cdot \varepsilon^*_{\lambda_l}(K)}{(K \cdot k_i)^2} \right] \times \left[\vec{Q}_{\text{eff}}(Q\bar{Q}'_{[81]}) \mathcal{A}^{(n,0)}_{\{[1],0,0,0\}}(r^{\not{i}}) + \vec{Q}_{\text{eff}}(Q\bar{Q}'_{[88]}) \mathcal{A}^{(n,0)}_{\{[8],0,0,0\}}(r^{\not{i}}) \right]$$

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- At $\left| \mathcal{A}^{(n+1,0)}_{\{[8],0,1,1\}}(r) \right|^2$, one such non-standard Eikonal integral looks like $\dfrac{(K \cdot k_k) k_{i,\mu}}{(k_k \cdot k_i)(K \cdot k_i)^2}$

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- Looking at their structure, we find they can be expressed as derivatives of the known standard ones. For instance,

$$\int d\Omega_i \frac{K\cdot k_k}{(k_k\cdot k_i)(K\cdot k_i)^2}k_{i,\mu} = -(K\cdot k_k)\frac{\partial}{\partial K_\mu}\left(\int d\Omega_i\frac{1}{(k_k\cdot k_i)(K\cdot k_i)}\right)$$

Extending FKS to quarkonium

- In general, for a single quarkonium with any quantum state, the Eikonal integral takes the form

$$k_k \cdot k_l \int d\Omega_i \frac{k_i^{\alpha_1} \ldots k_i^{\alpha_{n_1-1}} k_i^{\beta_1} \ldots k_i^{\beta_{n_2-1}}}{(k_k \cdot k_i)^{n_1} (k_l \cdot k_i)^{n_2}}, \quad n_1, n_2 \geq 1$$

- In addition to these counter terms, we have additional singularities from LDME renormalisation for the P-waves - Need counter term for them as well.
- For example, for $\left({}^1P_1^{[8]}\right)$ state, the counter term looks like

$$\frac{\alpha_s}{2\pi} d\phi_{n-1}(\dot{r}^{\not{k}}) \frac{J^{n_L^{(B)}}}{\mathcal{N}(\dot{r}^{\not{k}})} \mathcal{G}(\dot{r}^{\not{k}}) \left[B_F \mathbb{M}^{(n-1,0)}(\dot{r}_1^{\not{k}}) + C_F \mathbb{M}^{(n-1,0)}(\dot{r}_2^{\not{k}})\right] \frac{8}{m_Q m_{\bar{Q}'}} \left(\frac{1}{\bar{\epsilon}} + \log \frac{\mu^2}{\mu^2_{\text{NRQCD}}}\right)$$

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- In addition to these counter terms, we have additional singularities from LDME renormalisation for the P-waves - Need counter term for them as well.

- For example, for $\left({}^1P_1^{[8]}\right)$ state, the counter term looks like

$$\frac{\alpha_s}{2\pi} d\phi_{n-1}(\dot{r}^{\natural}) \frac{J^{n_L^{(B)}}}{\mathcal{N}(\dot{r}^{\natural})} \mathcal{G}(\dot{r}^{\natural}) \left[B_F \mathbb{M}^{(n-1,0)}(\dot{r}_1^{\natural}) + C_F \mathbb{M}^{(n-1,0)}(\dot{r}_2^{\natural}) \right] \frac{8}{m_Q m_{\bar{Q}'}} \left(\frac{1}{\bar{\epsilon}} + \log \frac{\mu^2}{\mu^2_{\text{NRQCD}}} \right)$$

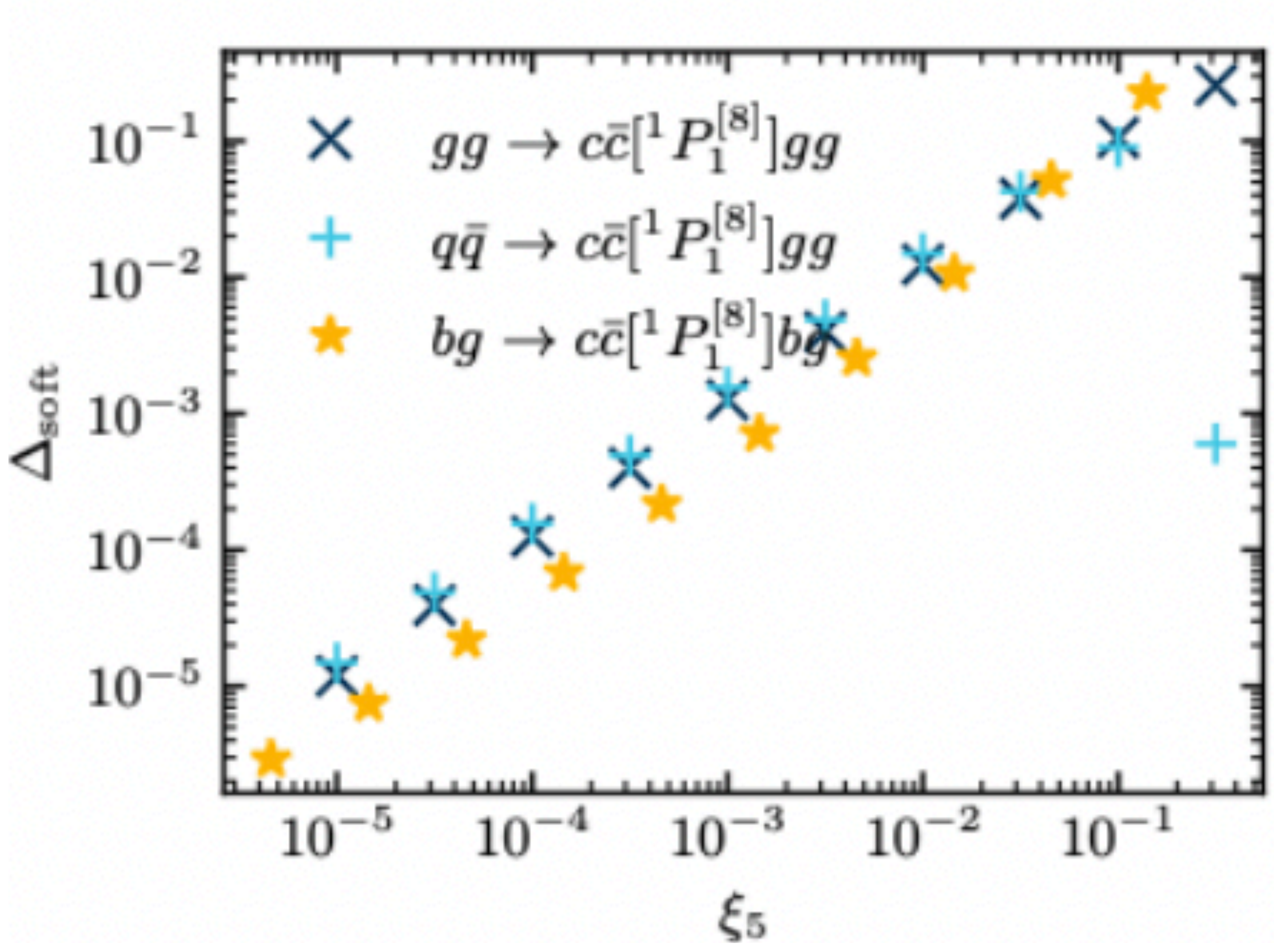
$$\langle \mathcal{O}^H_{{}^1S_0^{[8]}} \rangle (\mu) = \langle \mathcal{O}^H_{{}^1S_0^{[8]}} \rangle + \frac{4\alpha_s}{3\pi m_Q m_{\bar{Q}'}} \left(\frac{1}{\bar{\epsilon}} + \log \frac{\mu^2}{\mu^2_{\text{NRQCD}}} \right) \times \left[\frac{C_F}{2N_c} \langle \mathcal{O}^H_{{}^1P_1^{[1]}} \rangle + B_F \langle \mathcal{O}^H_{{}^1P_1^{[8]}} \rangle \right],$$

$$\langle \mathcal{O}^H_{{}^1S_0^{[1]}} \rangle (\mu) = \langle \mathcal{O}^H_{{}^1S_0^{[1]}} \rangle + \frac{4\alpha_s}{3\pi m_Q m_{\bar{Q}'}} \left(\frac{1}{\bar{\epsilon}} + \log \frac{\mu^2}{\mu^2_{\text{NRQCD}}} \right) \times \left[\langle \mathcal{O}^H_{{}^1P_1^{[8]}} \rangle \right],$$

Validation

- Together, these integrated counter terms, along with collinear and soft-collinear c.t for elementary particles, the singularities cancels out with those of virtual corrections.
- Validation
  - The poles are checked and cancel explicitly
  - To check local counter term

$$\Delta_{\text{soft}} = \left| \frac{\mathbb{M}^{(n,0)}(\dot{r}) - \lim_{k_i \to 0} \mathbb{M}^{(n,0)}(\dot{r})}{\mathbb{M}^{(n,0)}(\dot{r})} \right| \propto \xi_i + \mathcal{O}(\xi_i^2),$$



Summary & Outlook

- Here we discuss subtraction method, specifically FKS subtraction method and how that can be successfully extended to quarkonium productions.
- At the moment we applied for the single quarkonium case along with any arbitrary elementary particle productions, that could be massive/massless or colored/colorless.
- Its implementation in MadGraph5_aMC@NLO is ongoing.
- What could be done in near future
    - Multiple quarkonium productions
    - For the complete NLO automation, we also need a formalism for loop corrections part.

Back up slide

One of the Eikonal integral

- For example, for $\int d\Omega_i \frac{(K\cdot k_k)k_{i,\mu}}{(k_k\cdot k_i)(K\cdot k_i)^2}$ if mass of particle k is 0, upto an overall factor

Divergent part

$$\left\{\frac{1}{2\epsilon^2}\frac{k_k^\mu}{k_k\cdot k_l}+\frac{1}{\epsilon}\left[\frac{k_k^\mu}{k_k\cdot k_l}\left(1-\log\left(\frac{k_k\cdot k_l}{E_k m_l}\right)-\frac{1}{2}\log\left(\frac{\xi_{cut}^2 s}{Q_{\rm ES}^2}\right)\right)-\frac{k_l^\mu}{m_l^2}\right]\right\}$$

Finite part

$$\sum_{i=1}^{3} T_{i,12}^{(0,m_l),\mu},$$

$$\begin{aligned}
T_{1,12}^{(0,m_l),\mu} = \frac{k_k^\mu}{k_k\cdot k_l}\Bigg\{&-\frac{\pi^2}{12}-\log\left(\frac{\xi_{cut}^2 s}{Q_{\rm ES}^2}\right)+\frac{1}{4}\log^2\left(\frac{\xi_{cut}^2 s}{Q_{\rm ES}^2}\right)+\log\left(\frac{k_k\cdot k_l}{E_k m_l}\right)\log\left(\frac{\xi_{cut}^2 s}{Q_{\rm ES}^2}\right)\\
&-\log\left(\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)+\frac{1}{2}\log^2\left(\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)-\frac{1}{4}\log^2\left(\frac{1+\beta_l}{1-\beta_l}\right)\\
&+\mathrm{Li}_2\left(1-\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)-\mathrm{Li}_2\left(1-\frac{E_kE_l\,(1+\beta_l)}{k_k\cdot k_l}\right)\\
&+\frac{k_k\cdot k_l}{k_k\cdot k_l-E_kE_l(1-\beta_l)}\log\left(\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)+\frac{E_kE_l(1+\beta_l)}{k_k\cdot k_l-E_kE_l(1+\beta_l)}\log\left(\frac{k_k\cdot k_l}{E_kE_l\,(1+\beta_l)}\right)
\end{aligned}$$

$$\begin{aligned}
T_{2,12}^{(0,m_l),\mu} &= \frac{k_l^\mu}{m_l^2}\Bigg\{\log\left(\frac{\xi_{cut}^2 s}{Q_{\rm ES}^2}\right)+\frac{m_l^2}{\beta_l E_l^2}\Bigg[-\frac{1}{1-\beta_l^2}\log\left(\frac{1+\beta_l}{1-\beta_l}\right)-\frac{E_kE_l}{k_k\cdot k_l-E_kE_l(1-\beta_l)}\log\left(\frac{k_k\cdot k_l}{E_kE_l(1-\beta_l)}\right)\\
&\quad+\frac{E_kE_l}{k_k\cdot k_l-E_kE_l(1+\beta_l)}\log\left(\frac{k_k\cdot k_l}{E_kE_l(1+\beta_l)}\right)\Bigg]\Bigg\},\\
T_{3,12}^{(0,m_l),\mu} &= \frac{\delta^{\mu 0}}{k_k\cdot k_l-E_kE_l\,(1-\beta_l)}\Bigg\{E_k\left[\log\left(\frac{E_kE_l\,(1+\beta_l)}{k_k\cdot k_l}\right)-\log\left(\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)\right]\\
&\quad+\frac{k_k\cdot k_l\,m_l^2}{E_l^3\beta_l\,(1-\beta_l^2)}\log\left(\frac{1+\beta_l}{1-\beta_l}\right)+\frac{E_k\left(E_l^2\beta_l\,(1+\beta_l)+m_l^2\right)}{E_l^2\,(k_k\cdot k_l-E_kE_l\,(1+\beta_l))}\\
&\quad\times\left[E_kE_l\left(\log\left(\frac{E_kE_l\,(1+\beta_l)}{k_k\cdot k_l}\right)-\log\left(\frac{k_k\cdot k_l}{E_kE_l\,(1-\beta_l)}\right)\right)+\frac{k_k\cdot k_l}{1+\beta_l}\log\left(\frac{1+\beta_l}{1-\beta_l}\right)\right]\Bigg\}. \qquad \text{(A.13)}
\end{aligned}$$