Fixed Order Calculations

part 1 & 2

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Terascale Monte Carlo School 2024

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Contents

- Perturbation theory
- Cross sections
- Total cross section – an example
- Histograms – an example
- Going beyond leading order
- Numerics
  - subtraction
  - slicing
- ... and some Gary Larson comic strips

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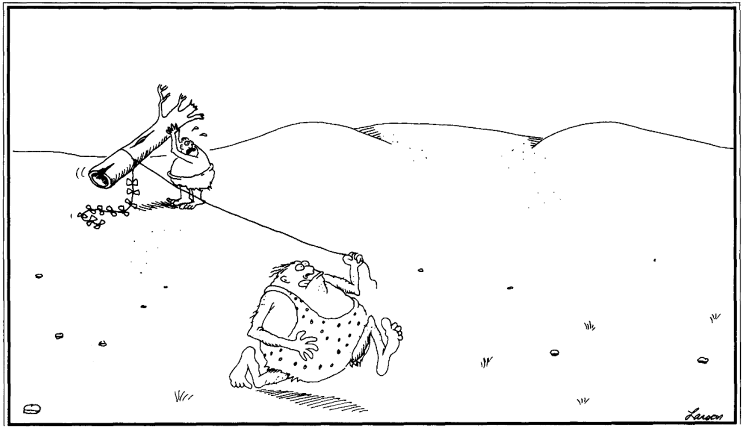
What is the purpose?

Show crucial steps on the road...

from here:



"Okay, Bob! Go! Go!"

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What is the purpose?

to here:

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Introduction

- Doing high-energy particle physics
- Common toolbox: perturbative quantum field theory
  - $\Rightarrow$ Perturbative: couplings considered small ($\ll 1$), Feynman diagrams
  - $\Rightarrow$ Quantum: even loop diagrams can appear
- Questions considered:
  - What can be calculated?
  - How this is done in practice?

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Defining perturbation theory

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Defining perturbation theory

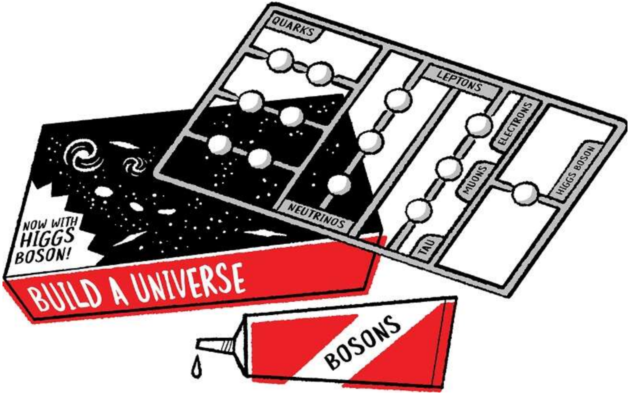
- Two important couplings for perturbations:
  - electric charge: e

$$e \Rightarrow \alpha_{em} = \frac{e^2}{4\pi}$$

  - strong coupling: g_s

$$g_s \Rightarrow \alpha_s = \frac{g_s^2}{4\pi}$$

$\Rightarrow$ Expanding in α_{em} and α_s



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Defining perturbation theory

Physical quantities are written as a series in these parameters:

$$\alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m+1}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m+2}\alpha_{\rm s}^{\rm n}(\dots) + \dots \quad \Rightarrow \text{EW corrections}$$

$$\alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+1}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+2}(\dots) + \dots \quad \Rightarrow \text{QCD corrections}$$

$$\left.\begin{aligned}
&\alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n}(\dots) + \\
&\alpha_{\rm em}^{\rm m+1}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+1}(\dots) + \\
&\alpha_{\rm em}^{\rm m+2}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m+1}\alpha_{\rm s}^{\rm n+1}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+2}(\dots) + \\
&\dots
\end{aligned}\right\} \Rightarrow \text{mixed corr.}$$

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Defining perturbation theory

- We focus on QCD corrections:

$$\alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+1}(\dots) + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+2}(\dots) + \dots$$

- If $\alpha_{\rm s} \ll 1$ including more and more terms theoretical precision increases
- N.B.:

$$\alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n}\underbrace{(\dots)}_{\not\sim \frac{1}{\alpha_{\rm s}^{\rm n}}} + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+1}\underbrace{(\dots)}_{\not\sim \frac{1}{\alpha_{\rm s}^{\rm n+1}}} + \alpha_{\rm em}^{\rm m}\alpha_{\rm s}^{\rm n+2}\underbrace{(\dots)}_{\not\sim \frac{1}{\alpha_{\rm s}^{\rm n+2}}} + \dots$$

$\Rightarrow$ Otherwise all orders are important (see resummation!)

What can be calculated?

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Cross sections

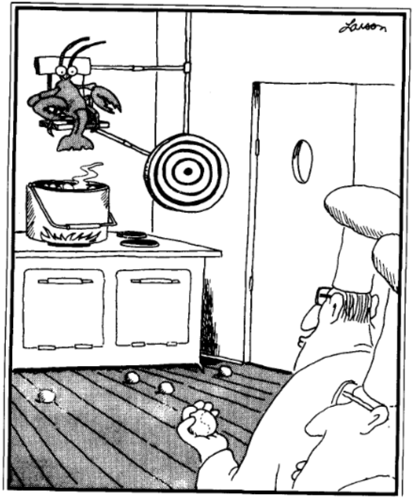
Cross sections

- Calculate (physical) observables represented by cross sections
- Easiest: total cross section (if defined):

$$\sigma = \underbrace{\frac{1}{2s}}_{\substack{\text{flux}\\ \text{factor}}} \int \underbrace{d\Phi_n}_{\substack{\text{phase}\\ \text{space}}} \underbrace{\left|\mathcal{M}_{a\,b\to n}\left(\Phi_n\right)\right|^2}_{\substack{\text{SME}\\ \text{aka. dynamics}}},$$

$s = 2p_a \cdot p_b$

- Note: only valid if initial states are identified (i.e. $e^+ e^-$ collisions)



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Cross sections

Ingredients:

- Phase space (PS) (in four space-time dimensions):

$$d\Phi_n^{(4)} = \left[\prod_{i=1}^{n} \frac{d^3\mathbf{p}_i}{(2\pi)^3 2E_i}\right](2\pi)^4\delta^{(4)}\left(p_a + p_b - \sum_{j=1}^{n} p_j\right) ,$$

$$m_i^2 = E_i^2 - \mathbf{p}_i^2 .$$

– Integration over PS can be done multiple ways:
  - DIY: early processes in `POWHEG-BOX`
  - Democratically generated by, e.g. `RAMBO`
  - Using some full-fledged generator, like `Kaleu`

- Many integration variables : $D_{\text{int}} = 3n - 4$

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Cross sections

- Dynamics
  - Squared Matrix Elements (SMEs) from Good Ol' Feynman diagrams
  - Model- and process-dependent
  - QFT under the hood
  - ⇒ Multileg and multiloop diagrams
- Nomenclature:

$$\alpha_{\text{em}}^{\mathsf{m}}\alpha_{\text{s}}^{\mathsf{n}}(\dots) + \alpha_{\text{em}}^{\mathsf{m}}\alpha_{\text{s}}^{\mathsf{n}+1}(\dots) + \alpha_{\text{em}}^{\mathsf{m}}\alpha_{\text{s}}^{\mathsf{n}+2}(\dots) + \dots$$

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Cross sections

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- Nomenclature:

$$\sigma = \underbrace{\alpha_{\mathrm{em}}^{\mathsf{m}} \alpha_{\mathrm{s}}^{\mathsf{n}} (\ldots)}_{\sigma_{\mathrm{LO}}} + \underbrace{\alpha_{\mathrm{em}}^{\mathsf{m}} \alpha_{\mathrm{s}}^{\mathsf{n}+1} (\ldots)}_{\sigma_{\mathrm{NLO}}} + \underbrace{\alpha_{\mathrm{em}}^{\mathsf{m}} \alpha_{\mathrm{s}}^{\mathsf{n}+2} (\ldots)}_{\sigma_{\mathrm{NNLO}}} + \ldots$$

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Cross sections

- Dynamics
  - Squared Matrix Elements (SMEs) from Good Ol' Feynman diagrams
  - Model- and process-dependent
  - QFT under the hood
  - ⇒ Multileg and multiloop diagrams
- Nomenclature:

$$\sigma = \sigma_{\mathrm{LO}} + \sigma_{\mathrm{NLO}} + \sigma_{\mathrm{NNLO}} + \dots$$

  - σ_{LO}: Leading Order (LO) (Born) cross section
  - σ_{NLO}: Next-to-Leading Order (NLO) cross section
  - σ_{NNLO}: Next-to-Next-to-Leading Order (NNLO) cross section

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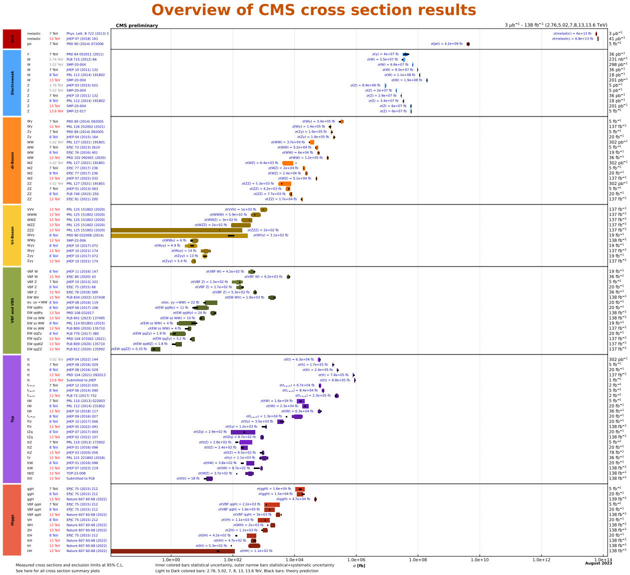
Cross sections



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Cross sections

Differential cross sections:

- Total cross section is a number
- More information in a distribution (more numbers):

$$\frac{\mathrm{d}\sigma}{\mathrm{d}X} = \frac{1}{2s} \int \mathrm{d}\Phi_n \left|\mathcal{M}_{a\,b\to n}\left(\Phi_n\right)\right|^2 \delta\left(X - \tilde{X}(\Phi_n)\right)$$

- X is the observable, can be expressed as a function of PS
  - Most energetic jet $p_\perp$, rapidity, etc.
  - C-parameter in $e^+ e^-$ collisions:

$$C(\Phi_n) = 3\left(1 - \sum_{i<j} \frac{s_{ij}^2}{(2p_i \cdot Q)(2p_j \cdot Q)}\right) , \quad Q = p_a + p_b$$

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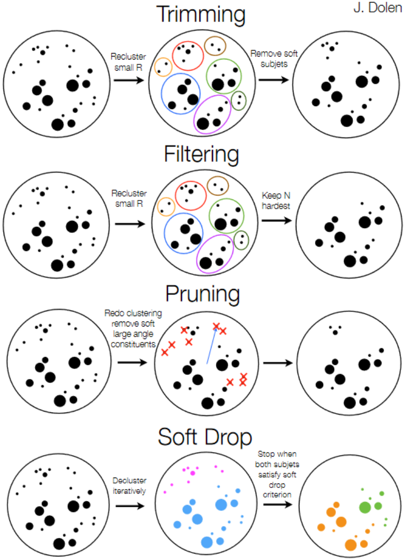
Cross sections

- Observables can be as complicated as they get

$\Rightarrow$ No way for (fully) analytic calculations

$\Rightarrow$ Cross sections obtained via Monte Carlo

- There is a reason we are here Today...



Total cross section – an example

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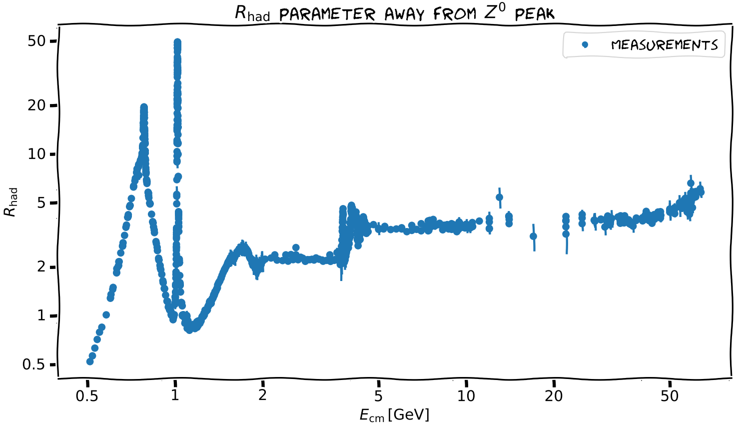
Total cross section – an example

$$R_{\text{had}} = \frac{\sigma_{e^+ e^- \to \text{hadrons}}}{\sigma_{e^+ e^- \to \mu^+ \mu^-}}$$



Total cross section – an example

$$R_{\rm had} = \frac{\sigma_{e^+e^-\to \rm hadrons}}{\sigma_{e^+e^-\to\mu^+\mu^-}}$$

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Total cross section – an example

$$R_{\text{had}} \approx \frac{\sigma^{\text{LO}}_{e^+ e^- \to \text{hadrons}}}{\sigma^{\text{LO}}_{e^+ e^- \to \mu^+ \mu^-}}$$

- Sticking to lowest order

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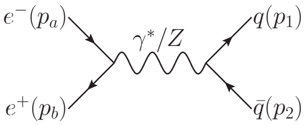
Total cross section – an example

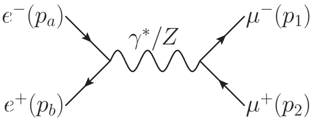
$$\mathrm{R_{had}} \approx \frac{\sum_{\mathrm{q}} \sigma^{\mathrm{LO}}_{\mathrm{e^+ e^- \to q\bar{q}}}}{\sigma^{\mathrm{LO}}_{\mathrm{e^+ e^-} \to \mu^+ \mu^-}}$$

- Sticking to lowest order
- Hadrons produced via quark-pair production

$$\sigma^{\mathrm{LO}}_{\mathrm{e^+ e^- \to q\bar{q}}} = \Bigg\{$$



$$\sigma^{\mathrm{LO}}_{\mathrm{e^+ e^-} \to \mu^+ \mu^-} = \Bigg\{$$



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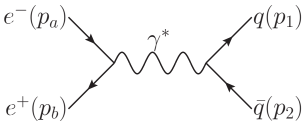
Total cross section – an example

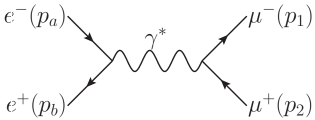
$$\mathrm{R_{had}} \approx \mathrm{R^{\gamma}_{had}} \approx \frac{\sum_q \sigma^{\mathrm{LO}}_{e^+e^- \to \gamma^* \to q\bar{q}}}{\sigma^{\mathrm{LO}}_{e^+e^- \to \gamma^* \to \mu^+\mu^-}}$$

$$\sigma^{\mathrm{LO}}_{e^+e^- \to \gamma^* \to q\bar{q}} = \left\{ \right.$$



- Sticking to lowest order
- Hadrons produced via quark-pair production
- $E_{cm} \ll m_Z$ photon exchange is good enough

$$\sigma^{\mathrm{LO}}_{e^+e^- \to \gamma^* \to \mu^+\mu^-} = \left\{ \right.$$



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Total cross section – an example

- Expression can be massaged to better fit numerical evaluation:

$$R^{\gamma}_{\mathrm{had}} = R^{\gamma}_{\mathrm{had}}(s) = \frac{1}{\sigma_0}\sum_{q}\frac{1}{2s}\int d\Phi_2 \left|\mathcal{M}_{e^+e^-\to\gamma^*\to q\bar{q}}\right|^2 ,$$

$$\sigma^{\mathrm{LO}}_{e^+e^-\to\gamma^*\to\mu^+\mu^-} = \frac{4\pi\alpha_{\mathrm{em}}^2}{3s} \equiv \sigma_0$$

- We have to evaluate a simple integral:

$$R^{\gamma}_{\mathrm{had}} = R^{\gamma}_{\mathrm{had}}(s) = \sum_{q} R^{\gamma}_{q}(s) ,$$

$$R^{\gamma}_{q}(s) = \frac{1}{\sigma_0}\frac{1}{2s}\int d\Phi_2 \left|\mathcal{M}_{e^+e^-\to\gamma^*\to q\bar{q}}\right|^2$$

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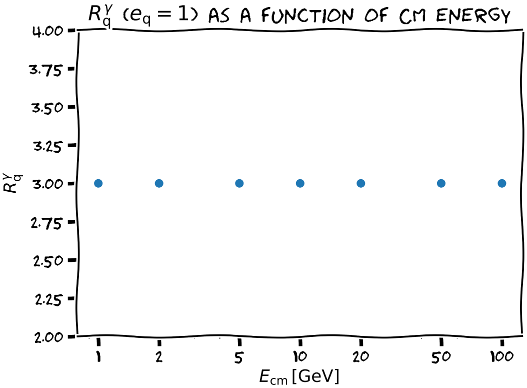
Total cross section – an example

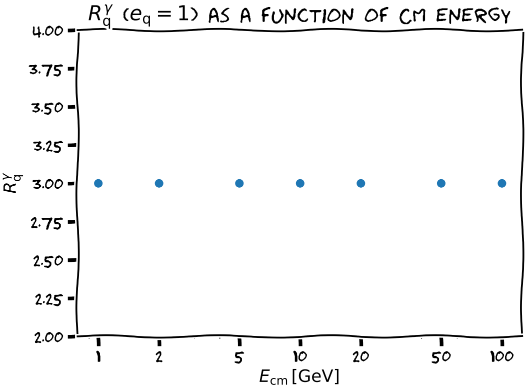
$$R^{\gamma}_{\mathrm{had}}(s) = \sum_{q} R^{\gamma}_{q}(s)$$



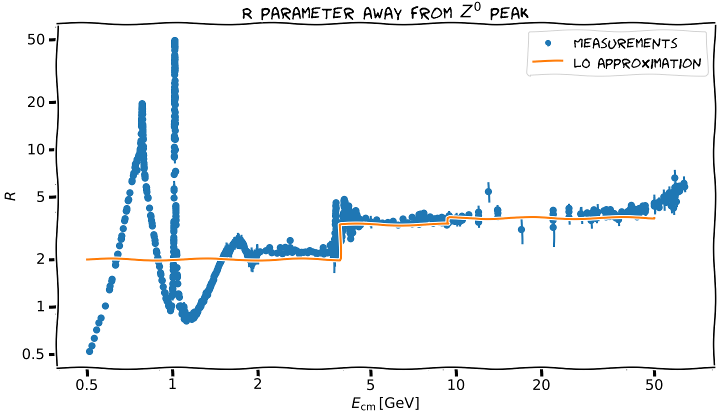
Total cross section – an example

$$R^{\gamma}_{\mathrm{had}} = N_c \sum_q e_q^2$$

q's	$R^{\gamma}_{\mathrm{had}}$
u, d, s	$2 \times \frac{1}{9} + 1 \times \frac{4}{9} = 2$
u, d, s, c	$2 \times \frac{1}{9} + 2 \times \frac{4}{9} = 3.333$
u, d, s, c, b	$3 \times \frac{1}{9} + 2 \times \frac{4}{9} = 3.666$



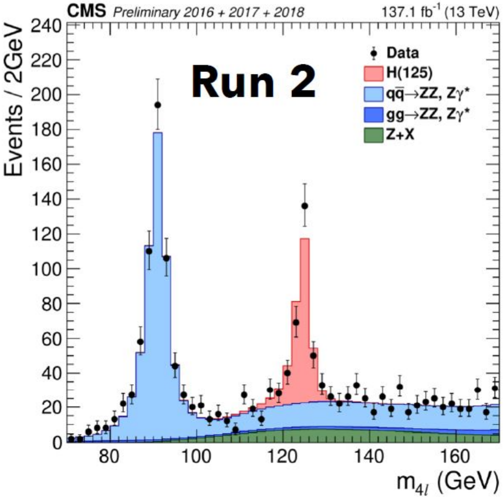
Total cross section – an example



Histograms – an example

Histograms – an example

- More numbers are more fun than one number
- Much higher stat is needed
  - Each bin is a "separate" calculation
  - Different bins can be populated at different rates (importance sampling)
- More complicated beyond LO
- More insight could be gained



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Histograms – an example

- Basic definition for differential cross section (wrt. X):

$$\frac{d\sigma}{dX} = \frac{1}{2s} \int d\Phi_n \left|\mathcal{M}_{a\,b\to n}\left(\Phi_n\right)\right|^2 \delta\left(X - \tilde{X}(\Phi_n)\right)$$

- In reality: histograms with finite bin width:

$$\frac{\Delta\sigma}{\Delta X} = \frac{1}{\Delta X}\frac{1}{2s} \int_{X\in[X,X+\Delta X]} d\Phi_n \left|\mathcal{M}_{a\,b\to n}\left(\Phi_n\right)\right|^2$$

  read: cross section contribution between X and $X + \Delta X$ divided by the width of the region.

- Total cross section (if exists):

$$\sigma = \int dX \frac{d\sigma}{dX} \Rightarrow \sum_X \frac{\Delta\sigma}{\Delta X}\Delta X$$

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Histograms – an example

- There can be variants:
  - weighing with observable:

$$X\frac{d\sigma}{dX} = \frac{1}{2s}\int d\Phi_n X\, |\mathcal{M}_{a\,b\to n}(\Phi_n)|^2\,\delta\left(X - \tilde{X}(\Phi_n)\right)$$

  - Normalizing with some total cross section:

$$\frac{1}{\sigma^{tot}}\frac{d\sigma}{dX} = \frac{1}{\sigma^{tot}}\frac{1}{2s}\int d\Phi_n\, |\mathcal{M}_{a\,b\to n}(\Phi_n)|^2\,\delta\left(X - \tilde{X}(\Phi_n)\right)$$

  - or both:

$$\frac{X}{\sigma^{tot}}\frac{d\sigma}{dX} = \frac{1}{\sigma^{tot}}\frac{1}{2s}\int d\Phi_n\, X\, |\mathcal{M}_{a\,b\to n}(\Phi_n)|^2\,\delta\left(X - \tilde{X}(\Phi_n)\right)$$

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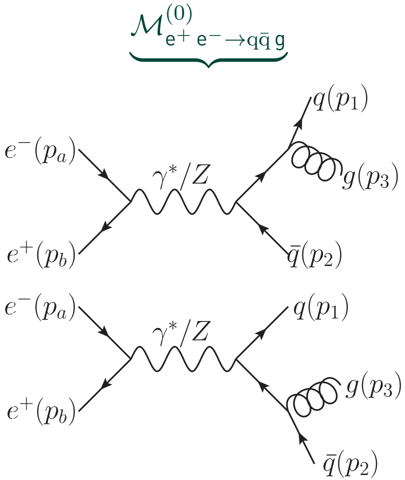
Histograms – an example

- Sticking to theme of $e^+ e^-$ collisions
- Using the C parameter:

$$C(\Phi_n) = 3\left(1 - \sum_{i<j} \frac{s_{ij}^2}{(2p_i \cdot Q)(2p_j \cdot Q)}\right)$$

- Notice: vanish for two-parton(-like) final state!

$\Rightarrow$ We need at least three partons!



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Histograms – an example

We calculate:

$$\frac{\mathsf{C}}{\sigma_{\text{had}}}\frac{\mathrm{d}\sigma}{\mathrm{d}\mathsf{C}} = \frac{1}{\sigma_{\text{had}}}\frac{1}{2\mathsf{s}}\int \mathrm{d}\Phi_3 \mathsf{C}(\Phi_3)\sum_{\mathrm{q}}\left|\mathcal{M}_{\mathsf{a}\,\mathsf{b}\to \mathrm{q}\bar{\mathrm{q}}\,\mathsf{g}}\left(\Phi_3\right)\right|^2 \delta\left(\mathsf{C} - \mathsf{C}(\Phi_3)\right) \,,$$

$$\sigma_{\text{had}} = \sigma^{\text{LO}}_{\mathsf{e}^+\,\mathsf{e}^-\to\text{hadrons}}$$

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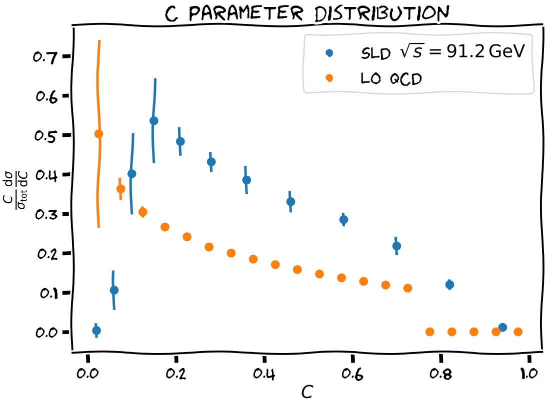
Histograms – an example



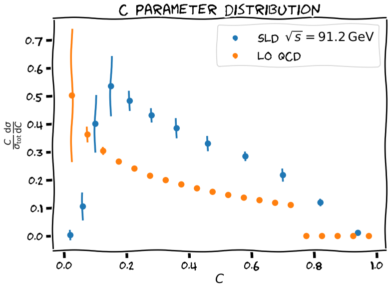
Histograms – an example

- Large diff. between data and pred.
  - LO only gives order of magnitude of cross section
  - Data: hadron level, pred.: parton level
  - Large hadronization corrections (Low CM energy!)

⇒ Need higher orders

⇒ Need hadronization (non-perturbative) corr.'s

⇒ At some places even all orders (resummation) are important!



Going beyond leading order

Going beyond leading order

- Perturbative expansion of matrix element for parton production:

$$\mathcal{M}_{\mathsf{e}^+\,\mathsf{e}^-\to\text{partons}} = \underbrace{\mathcal{M}^{(0)}_{\mathsf{e}^+\,\mathsf{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}}}_{\mathcal{O}(\alpha_\mathrm{s}^0)} + \underbrace{\mathcal{M}^{(0)}_{\mathsf{e}^+\,\mathsf{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}\,\mathsf{g}}}_{\mathcal{O}(\alpha_\mathrm{s})} + \ldots$$

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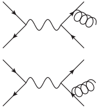

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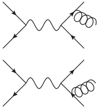
Going beyond leading order

- Perturbative expansion of matrix element for parton production:

$$\mathcal{M}_{e^+e^-\to\text{partons}} = \underbrace{\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}}} + \underbrace{\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}g}} + \dots$$



- Tempting to calculate corrections to R_{had}:

$$R_q^{\gamma,(1)} = \frac{1}{\sigma_0}\frac{1}{2s}\int d\Phi_3 \left|\mathcal{M}_{e^+e^-\to q\bar{q}g}\right|^2 .$$

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Going beyond leading order

Total cross section:

```
430.282664 +/- 113.967916
863.479534 +/- 416.143910
2153.29605 +/- 1523.17197
1693.97151 +/- 1142.45845
1397.71728 +/- 913.977829
1214.47253 +/- 761.770102
1077.28686 +/- 652.998983
1001.59986 +/- 571.960136
914.445041 +/- 508.417978
843.204778 +/- 457.580479
```

Diverges!

C-parameter calculation:

```
8.91493075 +/- 0.132625120
8.79626957 +/- 0.865028702E-1
8.72411096 +/- 0.622823457E-1
8.71186893 +/- 0.511833350E-1
8.70314723 +/- 0.439469194E-1
8.69395207 +/- 0.387525765E-1
8.69173048 +/- 0.357525446E-1
8.68077874 +/- 0.326236901E-1
8.66464537 +/- 0.298701218E-1
8.63943313 +/- 0.276904964E-1
```

Converges!

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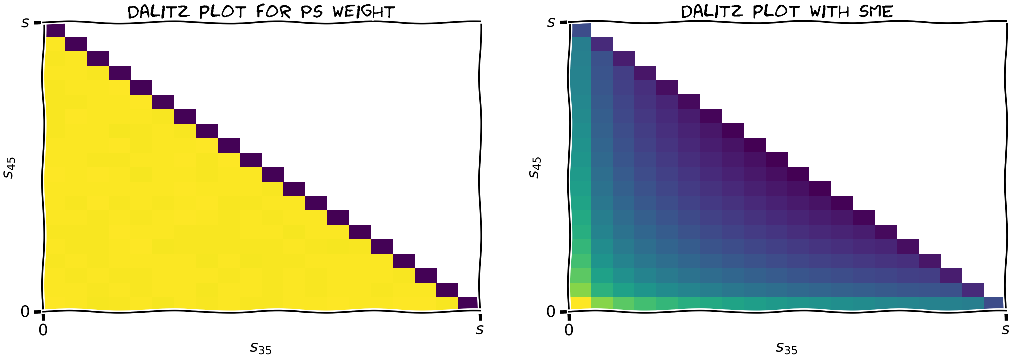
Going beyond leading order

What is singular? Take a look at the Dalitz plots:



Note: when weighing with SME, actually $\log |\mathcal{M}|^2$ was used!

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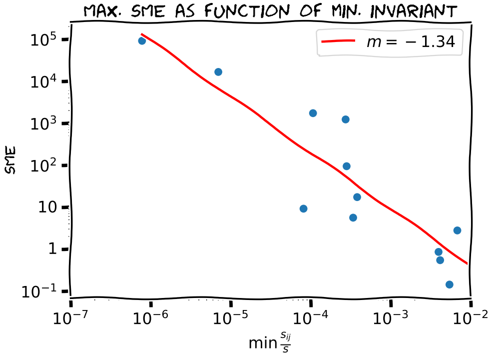
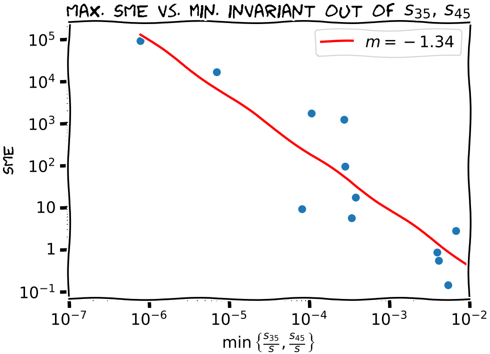
Going beyond leading order





as function of $\min_{i,j} \frac{s_{ij}}{s}$

as function of $\min \left\{ \frac{s_{13}}{s}, \frac{s_{23}}{s} \right\}$

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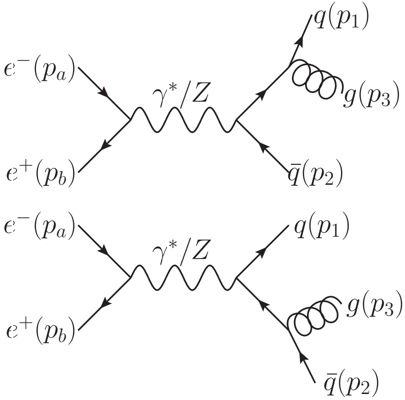
Going beyond leading order

$$\frac{1}{(p_1+p_3)^2} = \frac{1}{s_{13}}\,,$$
$$\frac{1}{(p_2+p_3)^2} = \frac{1}{s_{23}}$$

$$s_{13} = E_1E_3(1-\cos\theta_{13})\,,$$
$$s_{23} = E_2E_3(1-\cos\theta_{23})$$



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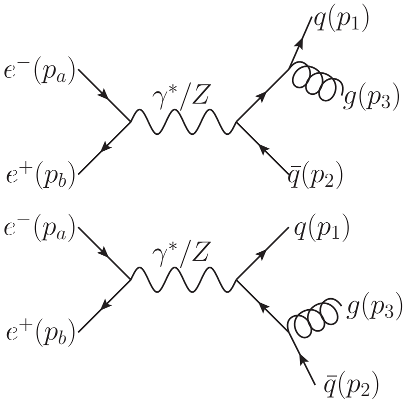
Going beyond leading order

$$\frac{1}{E_i E_j (1-\cos\theta_{ij})} \to \infty$$

$$\begin{cases} E_i \to 0 & \Rightarrow \quad \text{i soft}, \\ E_j \to 0 & \Rightarrow \quad \text{j soft}, \\ \theta_{ij} \to 0 & \Rightarrow \quad \text{i, j collinear} \end{cases}$$



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Going beyond leading order

How can this be made finite?

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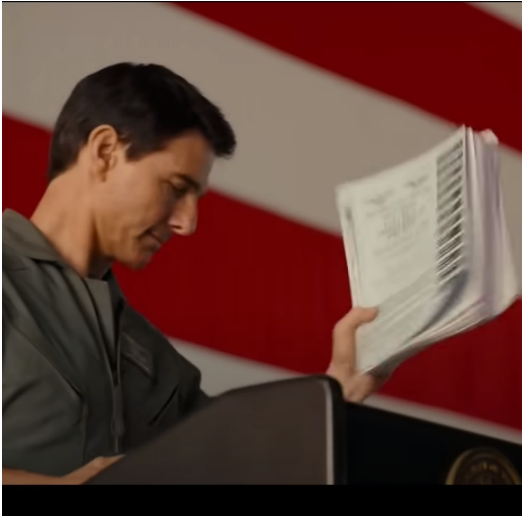
Going beyond leading order

How can this be made finite?



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Going beyond leading order

How can this be made finite?

- We are doing QFT

Going beyond leading order

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- We are doing QFT

$\Rightarrow$ Have tree diagrams

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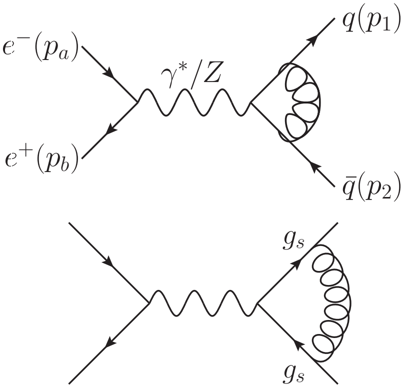
Going beyond leading order

How can this be made finite?

- We are doing QFT

$\Rightarrow$ Have tree diagrams

$\Rightarrow$ But also have loop diagrams!



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Going beyond leading order

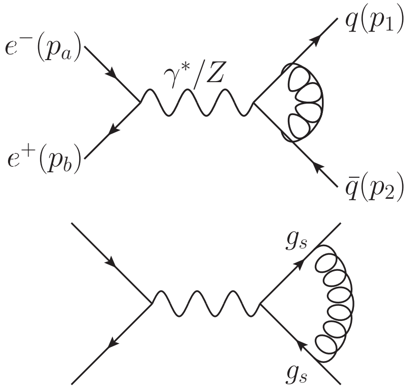
How can this be made finite?

- We are doing QFT

⇒ Have tree diagrams

⇒ But also have loop diagrams!

- Also, we do perturbation theory!



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Going beyond leading order

How can this be made finite?

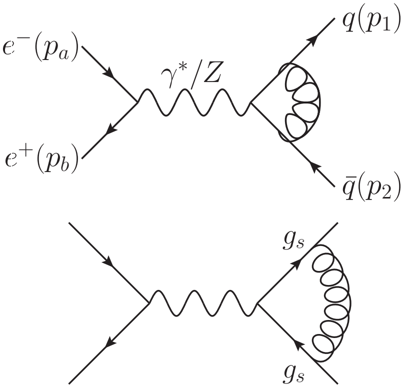
- We are doing QFT

⇒ Have tree diagrams

⇒ But also have loop diagrams!

- Also, we do perturbation theory!

⇒ All contributions at given order count!



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Going beyond leading order

- Perturbative expansion of matrix element becomes:

$$\mathcal{M}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{partons}} = \underbrace{\mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}}}_{\mathcal{O}(\alpha_\mathrm{s}^0)} + \underbrace{\mathcal{M}^{(1)}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}} + \mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}\,\mathrm{g}}}_{\mathcal{O}(\alpha_\mathrm{s})} + \ldots$$

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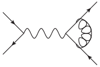
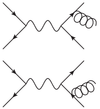
Going beyond leading order

- Perturbative expansion of matrix element becomes:

$$\mathcal{M}_{\mathrm{e}^+\,\mathrm{e}^- \to \mathrm{partons}} = \underbrace{\mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^- \to \mathrm{q}\,\bar{\mathrm{q}}}} + \underbrace{\mathcal{M}^{(1)}_{\mathrm{e}^+\,\mathrm{e}^- \to \mathrm{q}\,\bar{\mathrm{q}}}} + \underbrace{\mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^- \to \mathrm{q}\,\bar{\mathrm{q}}\,\mathrm{g}}} + \ldots$$





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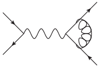
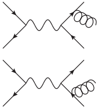
Going beyond leading order

- Perturbative expansion of matrix element becomes:

$$\mathcal{M}_{e^+e^-\to\text{partons}} = \underbrace{\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}}} + \underbrace{\mathcal{M}^{(1)}_{e^+e^-\to q\bar{q}}} + \underbrace{\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}g}} + \dots$$





- We need the SME to calculate cross section:

$$\left|\mathcal{M}_{e^+e^-\to\text{partons}}\right|^2 = \underbrace{\left|\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}}\right|^2}_{\mathcal{O}(\alpha_s^0)} +$$

$$+ \underbrace{2\text{Re}\left[\mathcal{M}^{(1)\dagger}_{e^+e^-\to q\bar{q}}\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}}\right] + \left|\mathcal{M}^{(0)}_{e^+e^-\to q\bar{q}g}\right|^2}_{\mathcal{O}(\alpha_s)} + \dots$$

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Going beyond leading order

Getting finite out of two infinite contributions:

$$\sigma_{\mathrm{NLO}} = \underbrace{2(\dots)\mathrm{Re}\int \mathrm{d}\Phi_2 \left[\mathcal{M}^{(1)\,\dagger}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}}\mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}}\right]}_{-\infty} + \underbrace{(\dots)\int \mathrm{d}\Phi_3 \left|\mathcal{M}^{(0)}_{\mathrm{e}^+\,\mathrm{e}^-\to\mathrm{q}\,\bar{\mathrm{q}}\,\mathrm{g}}\right|^2}_{+\infty} = \mathrm{finite}$$

Having different multiplicities!

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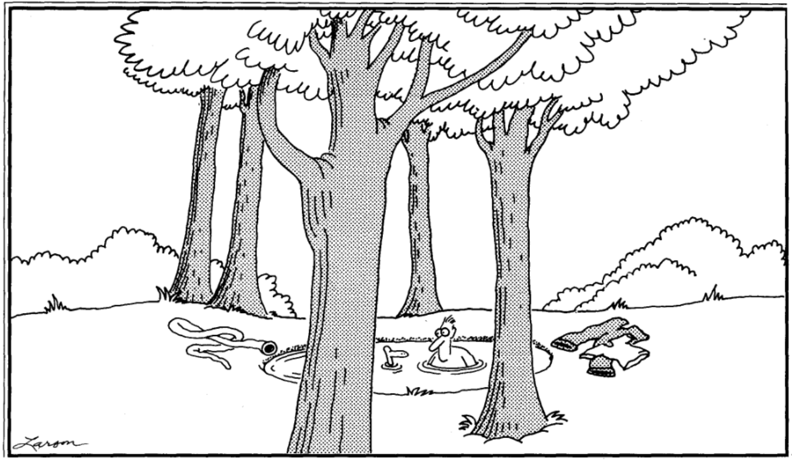
Going beyond leading order



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Going beyond leading order

- Impossible to combine contributions

⇒ How to get rid of singularities?

- Traditional way: convert infinities to poles:

$$\infty \quad \to \quad \lim_{\epsilon\to 0}\frac{1}{\epsilon^{\mathsf{n}}}\,, \quad \mathsf{n} > 0$$

- Done: change PS dimension:

$$\mathrm{d}\Phi_{\mathsf{n}}^{(4)} \to \mathrm{d}\Phi_{\mathsf{n}}^{(\mathsf{d})}$$

⇒ No numerics possible!

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Going beyond leading order

$$\mathcal{V} = 2\mathrm{Re}\left[\mathcal{M}^{(1)\,\dagger}_{\mathsf{e}^+\,\mathsf{e}^-\to\mathsf{q}\,\bar{\mathsf{q}}}\mathcal{M}^{(0)}_{\mathsf{e}^+\,\mathsf{e}^-\to\mathsf{q}\,\bar{\mathsf{q}}}\right]\,, \quad \mathcal{R} = \left|\mathcal{M}^{(0)}_{\mathsf{e}^+\,\mathsf{e}^-\to\mathsf{q}\,\bar{\mathsf{q}}\,\mathsf{g}}\right|^2\,,$$

$$\sigma^{\mathrm{V}}_{\mathrm{NLO}} = \frac{1}{2\mathsf{s}}\int \mathrm{d}\Phi_2^{(\mathsf{d})}\mathcal{V} = \sigma^{\mathrm{LO},(\mathsf{d})}_{\mathrm{had}}\mathsf{C_F}\frac{\alpha_{\mathrm{s}}}{\pi}\left\{-\frac{1}{\epsilon^2}-\frac{3}{2\epsilon}-4+\frac{7\pi^2}{12}+\mathcal{O}(\epsilon)\right\}\,,$$

$$\sigma^{\mathrm{R}}_{\mathrm{NLO}} = \frac{1}{2\mathsf{s}}\int \mathrm{d}\Phi_2^{(\mathsf{d})}\mathcal{R} = \sigma^{\mathrm{LO},(\mathsf{d})}_{\mathrm{had}}\mathsf{C_F}\frac{\alpha_{\mathrm{s}}}{\pi}\left\{+\frac{1}{\epsilon^2}+\frac{3}{2\epsilon}+\frac{19}{4}-\frac{7\pi^2}{12}+\mathcal{O}(\epsilon)\right\}$$

$$\sigma_{\mathrm{NLO}} = \sigma^{\mathrm{LO}}_{\mathrm{had}}\frac{\alpha_{\mathrm{s}}}{\pi}\mathsf{C_F}\frac{3}{4} = \sigma^{\mathrm{LO}}_{\mathrm{had}}\frac{\alpha_{\mathrm{s}}}{\pi} \quad \Rightarrow \quad \sigma^{\mathrm{NLO}} = \sigma_{\mathrm{LO}}+\sigma_{\mathrm{NLO}} = \sigma^{\mathrm{LO}}_{\mathrm{had}}\left(1+\frac{\alpha_{\mathrm{s}}}{\pi}\right)$$

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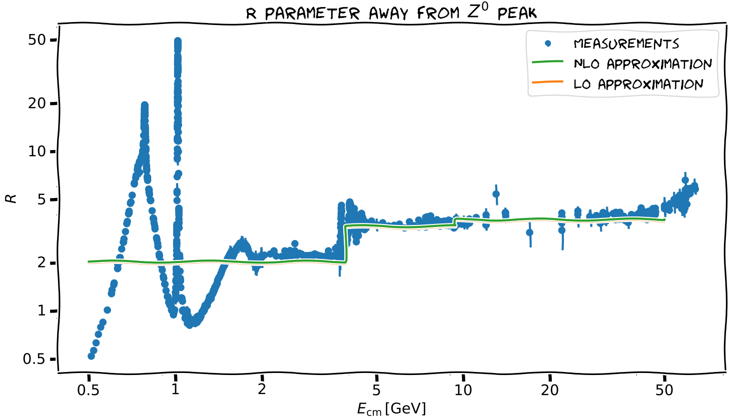
Going beyond leading order



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Numerics

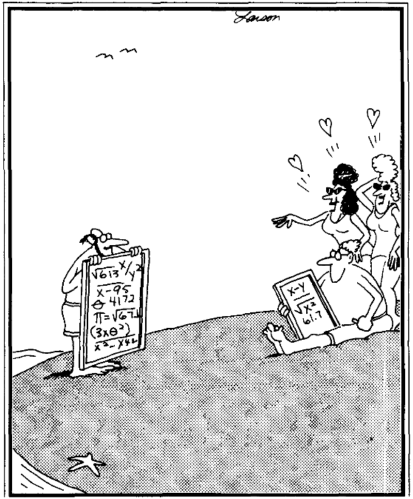
Numerics

- Complicated observables
- Complicated dynamics

$\Rightarrow$ Analytical calculation cannot be pushed through

$\Rightarrow$ We need numerics (for the real emission part)!

- Two mature approaches:
  - Subtraction
  - Slicing
- Zoltán Nagy: "We solve a math problem"



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Numerics – subtraction

Essence of subtraction methods:

Add zero in a clever(ish) way

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Numerics – subtraction

Consider an expression where only the sum is finite:

$$\mathsf{I} = \lim_{\epsilon \to 0} \left[\int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} \mathsf{F}(\mathsf{x}) - \frac{1}{\epsilon} \mathsf{F}(0) \right] = \text{finite}$$

We have the same situation as in the NLO (and beyond) case:

$$\mathsf{I} = \underbrace{\lim_{\epsilon \to 0} \int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} \mathsf{F}(\mathsf{x})}_{\infty} - \underbrace{\lim_{\epsilon \to 0} \frac{1}{\epsilon} \mathsf{F}(0)}_{\infty} = \text{finite}$$

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Numerics – subtraction

Guess the singular behavior of the integrand:

$$\lim_{x\to 0}\frac{1}{x^{1-\epsilon}}F(x)\sim\lim_{x\to 0}\frac{1}{x^{1-\epsilon}}F(0)$$

If this singular behavior is subtracted the difference is finite and integrable in $d=4$:

$$\lim_{\epsilon\to 0}\int_0^1\frac{dx}{x^{1-\epsilon}}\left[F(x)-F(0)\right]=\int_0^1\frac{dx}{x}\left[F(x)-F(0)\right]=\text{finite}$$

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Numerics – subtraction

But this is all wrong!

New term appears in cross section $\Rightarrow$ result is not physical

$$I = \lim_{\epsilon\to0}\left[\int_0^1 \frac{dx}{x^{1-\epsilon}}F(x) - \frac{1}{\epsilon}F(0)\right] \Rightarrow$$
$$\Rightarrow \int_0^1 \frac{dx}{x}\left[F(x) - F(0)\right] - \lim_{\epsilon\to0}\frac{1}{\epsilon}F(0) \neq I$$

First term became regular, but second did not!

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Numerics – subtraction

Have to add zero!

$$\underbrace{-\int_0^1 \frac{\mathrm{d}x}{x^{1-\epsilon}} F(0) + F(0) \int_0^1 \frac{\mathrm{d}x}{x^{1-\epsilon}}}_{0} = -\int_0^1 \frac{\mathrm{d}x}{x^{1-\epsilon}} F(0) + F(0) \frac{x^\epsilon}{\epsilon}\bigg|_0^1 = -\int_0^1 \frac{\mathrm{d}x}{x^{1-\epsilon}} F(0) + \frac{1}{\epsilon} F(0)$$

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Numerics – subtraction

$$\mathsf{I} = \lim_{\epsilon \to 0} \left[\int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} \mathsf{F}(\mathsf{x}) - \frac{1}{\epsilon} \mathsf{F}(0) \right]$$

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Numerics – subtraction

$$I = \lim_{\epsilon \to 0} \left[\int_0^1 \frac{dx}{x^{1-\epsilon}} F(x) \underbrace{- \int_0^1 \frac{dx}{x^{1-\epsilon}} F(0) + F(0) \int_0^1 \frac{dx}{x^{1-\epsilon}}}_{0} - \frac{1}{\epsilon} F(0) \right]$$

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Numerics – subtraction

$$\mathsf{I} = \lim_{\epsilon \to 0} \left[\int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} \mathsf{F}(\mathsf{x}) - \int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} \mathsf{F}(0) + \frac{1}{\epsilon} \mathsf{F}(0) - \frac{1}{\epsilon} \mathsf{F}(0) \right]$$

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Numerics – subtraction

$$I = \lim_{\epsilon \to 0} \int_0^1 \frac{dx}{x^{1-\epsilon}} \left[F(x) - F(0)\right]$$

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Numerics – subtraction

$$I = \int_0^1 \frac{dx}{x} \left[F(x) - F(0)\right] = \text{finite}$$

Numerics – subtraction

Properties of subtractions:

- For (fully local) subtractions the integral will not change
- Have to figure out singular structure
- Reduced analytical integrations
  - Integrated subterms and loop, like Catani-Seymour
  - Virtual contribution, like HELAC
- Only the full sum of contributions is physical (true for all $N^{x}LO$ calculations)!

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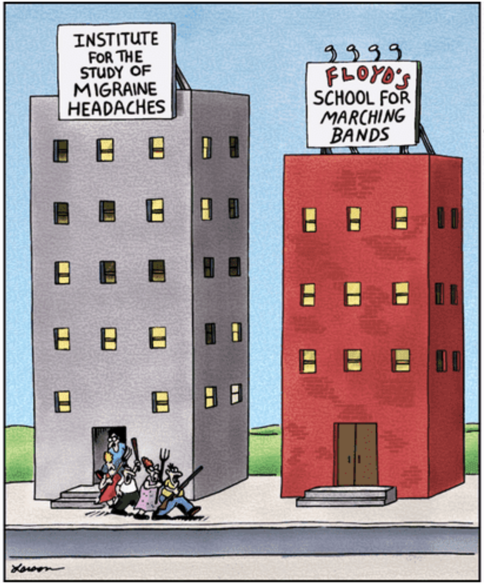
Numerics – subtraction



Numerics – slicing

Essence of slicing methods:

Select quantity to partition phase space and approximate for small values.

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Numerics – slicing

- Consider the previous toy example:

$$\mathsf{I} = \lim_{\epsilon\to 0}\left[\int_0^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}}\mathsf{F}(\mathsf{x}) - \frac{1}{\epsilon}\mathsf{F}(0)\right] = \text{finite}$$

- Partition integration ($\delta \ll 1$):

$$\mathsf{I} = \lim_{\epsilon\to 0}\left[\int_\delta^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}}\mathsf{F}(\mathsf{x}) + \int_0^\delta \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}}\mathsf{F}(\mathsf{x}) - \frac{1}{\epsilon}\mathsf{F}(0)\right]$$

- For small x values we approximate F(x):

$$\mathsf{I} \approx \lim_{\epsilon\to 0}\left[\int_\delta^1 \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}}\mathsf{F}(\mathsf{x}) + \mathsf{F}(0)\int_0^\delta \frac{\mathrm{d}\mathsf{x}}{\mathsf{x}^{1-\epsilon}} - \frac{1}{\epsilon}\mathsf{F}(0)\right]$$

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Numerics – slicing

- Due to approximation that term is easier to calculate:

$$I \approx \lim_{\epsilon\to 0}\left[\int_\delta^1 \frac{dx}{x^{1-\epsilon}} F(x) + F(0)\frac{1}{\epsilon}\delta^\epsilon - \frac{1}{\epsilon}F(0)\right]$$

- δ is small and $\epsilon \to 0$:

$$\delta^\epsilon = 1 + \epsilon \log\delta + \mathcal{O}\left(\epsilon^2\right)$$

$$I \approx \lim_{\epsilon\to 0}\left[\int_\delta^1 \frac{dx}{x^{1-\epsilon}} F(x) + F(0)\log\delta \underbrace{+\frac{1}{\epsilon}F(0) - \frac{1}{\epsilon}F(0)}_{0}\right]$$

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Numerics – slicing

- Remaining terms are finite:

$$I \approx \lim_{\epsilon\to 0}\left[\int_{\delta}^{1}\frac{dx}{x^{1-\epsilon}}F(x)+F(0)\log\delta\right]$$

$$I \approx \int_{\delta}^{1}\frac{dx}{x}F(x)+F(0)\log\delta$$

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Numerics – slicing

Properties of slicing:

- An approximation to the original problem
- Several variants, depending on observable:
  - $q_\perp$ slicing
  - Jettiness slicing
  - ...
- Care is needed because approximation
- For certain observables dropped pieces can be large

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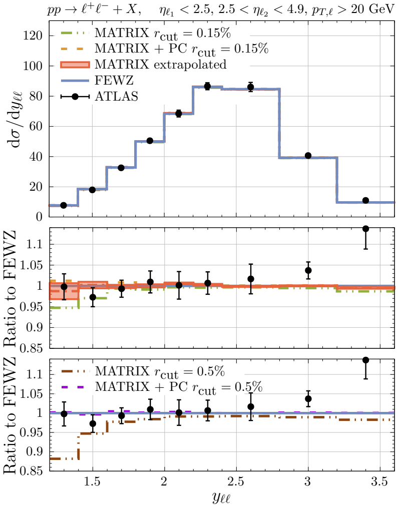
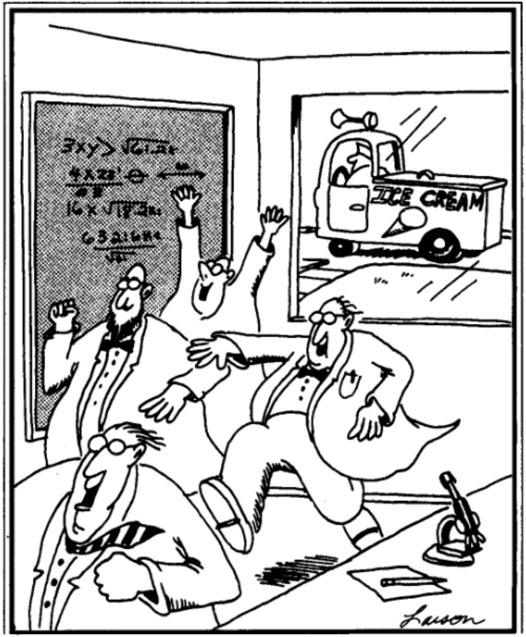
Numerics – slicing

- There can be special observables sensitive to slicing
- Extra care is needed to consider neglected terms

One example:

- Lepton-pair production in pp collisions
- Using symmetric lepton $p_\perp$ cuts
- One central, one forward lepton





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Thank you for your attention!