

# Pseudoscalar Quarkonium Hadroproduction and Decay up to Two Loops

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# My PhD thesis

- Title: Pseudoscalar Quarkonium Hadroproduction and Decay up to Two Loops
- PhD supervisor: Jean-Philippe Lansberg
- Institute: IPN Orsay, Theory Division (Head: Michael Urban), IJCLab, Theory Pole (Head: Samuel Wallon)
- Collaborators: Samuel Abreu (CERN), Matteo Beccetti (Torino), Claude Duhr (Bonn), Hua-Sheng Shao (Jussieu), ...
- Now: → Post-Doc at Institute for Theoretical Particle Physics (TTP), Karlsruhe Institute of Technology (KIT)

# Outline

Introduction

Part I: Quarkonium phenomenology at NLO

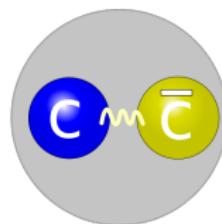
Part II: Two-loop master integrals and form-factors

Part III: Decay of pseudo-scalar to di-photon at NNLO accuracy

# Introduction

# Introduction: What is a Quarkonium?

- similar to positronium bound state  $e^+e^-$  in QED
- bound state of heavy **quark** and its **anti-quark** in QCD, e.g. Charmonium (charm quark) and Bottomonium (bottom quark)



[Figure from Wikipedia 'Quarkonium']

- Toponium ( $t\bar{t}$ ) bound state: high mass of top quark  $\rightarrow$  decays via weak interaction before formation of bound state
- for light quarks: mixing between (u,d,s) quarks due to low mass difference  $\rightarrow \pi$ -meson, the  $\rho$ -meson and the  $\eta$ -meson

# Motivation: Why study Quarkonia?

- charmonium production allows us to probe QCD at its interplay between the perturbative and non-perturbative regimes
- deeper understanding of confinement (production mechanism)
- access to spin/momentum distribution of gluons in protons  
→ use quarkonia to constrain the gluon PDFs in the proton (see Part I)
- it is interesting to assess the convergence of perturbative expansion in  $\alpha_s$  where  $\alpha_s(m_c) \sim 0.34$  and  $\alpha_s(m_b) \sim 0.22$  (see Part III)

# Part I

## Quarkonium phenomenology at NLO

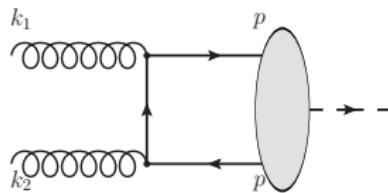
based on arXiv:1907.01400 and arXiv:2012.00702

## fixed-order calculation in a nutshell

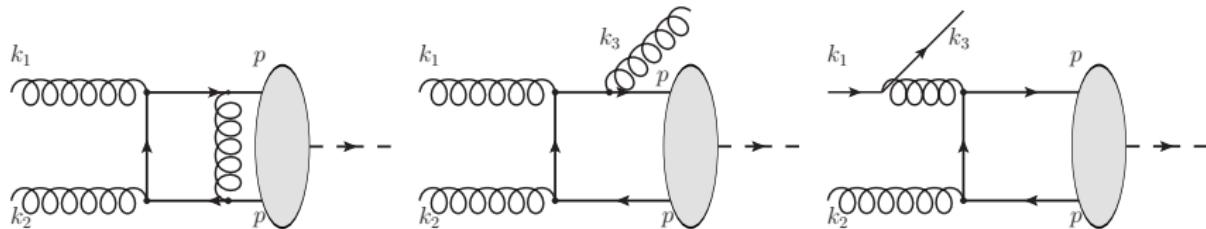
- fixed-order calculation: consider all contributions at given order in strong coupling  $\alpha_s$

$$\hat{\sigma} = \left(\frac{\alpha_s}{\pi}\right)^q \left[ \hat{\sigma}^{\text{LO}} + \left(\frac{\alpha_s}{\pi}\right) \hat{\sigma}^{\text{NLO}} + \left(\frac{\alpha_s}{\pi}\right)^2 \hat{\sigma}^{\text{NNLO}} + \dots \right] \quad (1)$$

- Leading Order (LO): first non-zero contribution in coupling



- Next-to-Leading Order (NLO): additional power of  $\alpha_s$

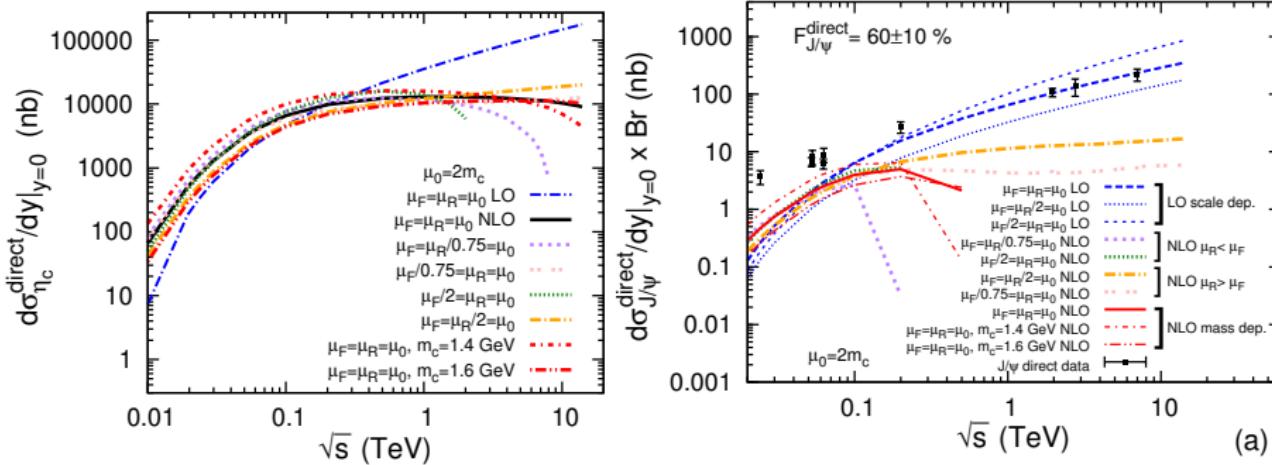


## fixed-order calculation in a nutshell

$$\sigma_{pp} = \sum_{ij} \int dx_1 dx_2 f_{i/p}(x_1, \mu_F) f_{j/p}(x_2, \mu_F) \hat{\sigma}_{ij}(\mu_R, \mu_F, \hat{s} = sx_1 x_2) \quad (2)$$

- artificial scales enter computation:
  - renormalisation scale  $\mu_R \rightarrow$  implicitly inside  $\alpha_s$  and explicitly in  $\hat{\sigma}_{ij}$
  - factorisation scale  $\mu_F \rightarrow$  implicitly inside PDF and explicitly in  $\hat{\sigma}_{ij}$
- a priori: no rigorous criterion for these scales  
→ scale uncertainties
  - scale uncertainties reduced at higher orders (e.g. NNLO and beyond)

# problem of negative cross-sections - $\eta_c$ and $J/\psi$ at NLO



comparison of  $\eta_c$  (left) and  $J/\psi$  (right) differential cross-sections at NLO with different scale choices of  $\mu_R$  and  $\mu_F$  with CTEQ6M

[Y. Feng, J.-P. Lansberg, J.X. Wang, Eur.Phys.J. C75 (2015) no.7, 313]

## the $\eta_c$ - a good gluon probe

- negative NLO cross-section unphysical (negative probability)
- implies that NLO correction parts are larger than LO

$$\sigma_{\text{LO}} \left( 1 + \underbrace{\frac{\alpha_s}{\pi} \delta_{\text{NLO}}}_{<-1} \right) < 0 \quad (3)$$

→ breakdown of perturbation theory?

Reminder for hadro-production:

	$\eta_Q$	$J/\psi$ and $\Upsilon$
QCD		

→ will study NLO correction to the **pseudo-scalar** ( $\eta_Q$ ) and will trace back origin of negative numbers

## partonic high-energy limit

The partonic high-energy limit is defined as taking  $\hat{\sigma}$  at  $\hat{s} \rightarrow \infty$  or equivalently  $z \rightarrow 0$  with  $z = \frac{M_Q^2}{\hat{s}}$ ,

### Definition

$$\lim_{z \rightarrow 0} \hat{\sigma}_{ab}^{\text{NLO}}(z) = C_{ab} \frac{\alpha_s}{\pi} \hat{\sigma}_0^{\text{LO}} \left( \log \frac{M^2}{\mu_F^2} + \hat{A} \right) \quad (4)$$

## partonic high-energy limit

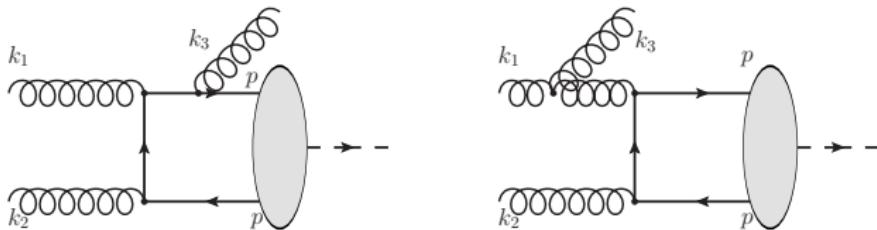
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- for  ${}^1S_0^{[1,8]}$ :  $\boxed{\hat{A} = A_{gg} = A_{qg} = -1}$
- for  $\mu_F = M$ , this limit is negative  $\rightarrow \propto -\frac{\alpha_s}{\pi} \hat{\sigma}_0^{\text{LO}}$
- limit enhanced (large weight) when gluon PDF is flat in low- $x$  region

# origin of negative numbers



- phase-space integration of real emission diagrams will reveal IR singularities → absorbed inside Parton Distribution Function

$$\lim_{z \rightarrow 0} \hat{\sigma}_{ab}^{\text{NLO}} = C_{ab} \frac{\alpha_s}{\pi} \hat{\sigma}_0^{\text{LO}} \left( \log \frac{M_Q^2}{\mu_F^2} + \hat{A} \right) \quad (5)$$

- If  $\left( \log \frac{M_Q^2}{\mu_F^2} + \hat{A} \right) < 0$  then **over-subtraction** from the AP-CT in  $\overline{\text{MS}}$ -scheme
- Problem:  $\hat{A}$  is **process-dependent** and thus cannot be compensated in a global manner via the **process-independent** DGLAP equations

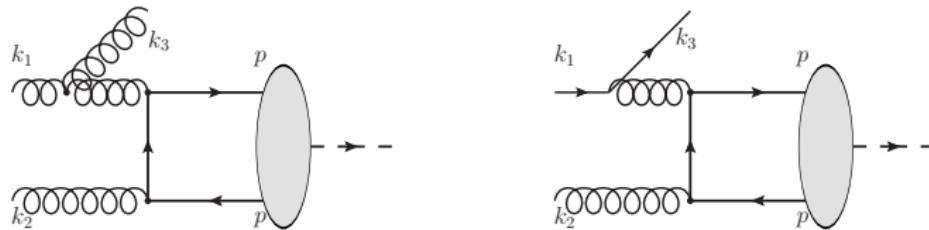
## a new scale prescription for $\mu_F$

- new scale prescription for  $\mu_F$ , [J.-P. Lansberg, Melih A. Ozcelik, Eur.Phys.J.C 81 (2021) 6, 497 (arXiv:2012.00702)]

$$\mu_F = \hat{\mu}_F = M e^{\hat{A}/2}$$

such that  $\left( \log \frac{M^2}{\mu_F^2} + \hat{A} \right) = 0 \rightarrow \lim_{z \rightarrow 0} \hat{\sigma}_{ab}^{\text{NLO}}(z) = 0.$

- Physics interpretation: absorption of all real emissions inside PDFs (resummation picture)



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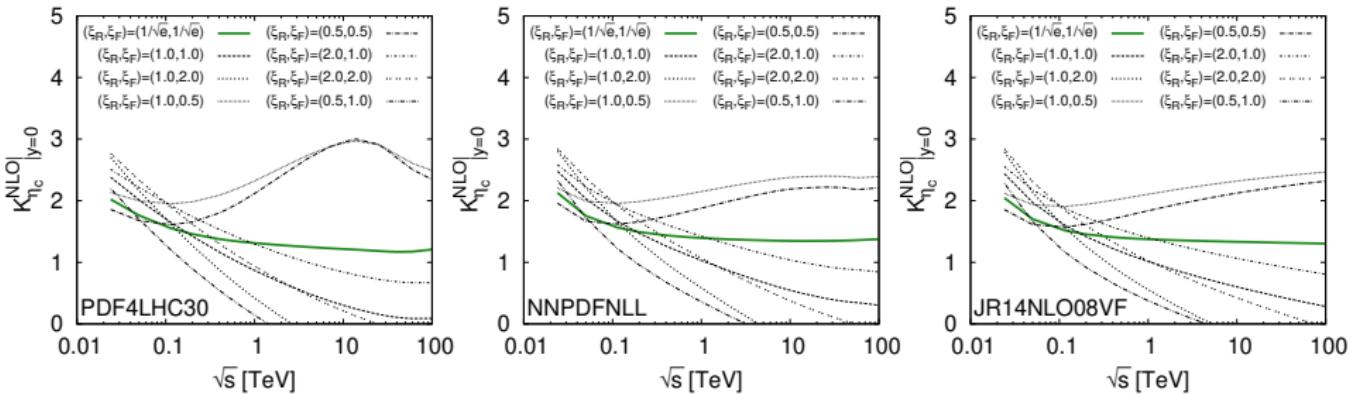
such that  $\left( \log \frac{M^2}{\mu_F^2} + \hat{A} \right) = 0 \rightarrow \lim_{z \rightarrow 0} \hat{\sigma}_{ab}^{\text{NLO}}(z) = 0$ .

- Physics interpretation: absorption of all real emissions inside PDFs (resummation picture)

for  $\eta_Q$  we have  $\hat{\mu}_F = \frac{M}{\sqrt{e}} = \begin{cases} 1.82 \text{GeV} & \text{for } \eta_c \text{ with } M = 3 \text{GeV} \\ 5.76 \text{GeV} & \text{for } \eta_b \text{ with } M = 9.5 \text{GeV} \end{cases}$

scale choice for  $\eta_Q$  are within typical bounds  $[\frac{M}{2}, 2M]$

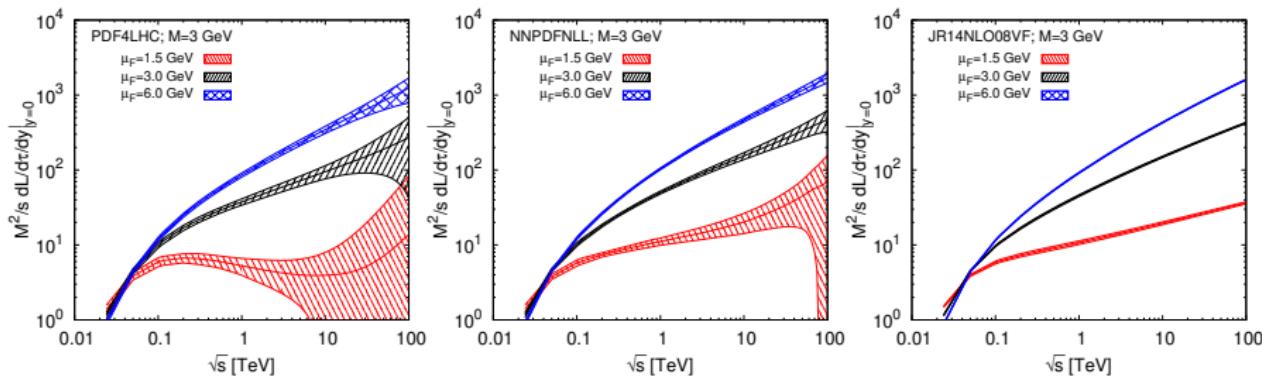
# $\frac{d\sigma}{dy} K\text{-factor for } \eta_c\text{-production at } y = 0$



- K-factor: assess perturbative convergence
- **new scale choice  $\hat{\mu}_F$  (green curve) ✓:**
  - perturbatively stable over energy range ✓
  - very similar results with different PDF parametrisation ✓
- other  $\mu_F$  scale choices:
  - not perturbative stable and negative results at large energy ✗
  - different results with different PDF parametrisation ✗

# PDFs at low scales

- charmonium production: low scales  $\rightarrow$  PDFs are close to initial parametrisation  $\rightarrow$  unconstrained due to lack of data
- luminosity plots,  $\frac{d\sigma^{\text{LO}}}{dy} \propto \frac{M^2}{s} \frac{\partial^2 \mathcal{L}}{\partial \tau \partial y} = \frac{M^2}{s} f_g(\sqrt{\tau} e^y, \mu_F) f_g(\sqrt{\tau} e^{-y}, \mu_F)$



$\rightarrow$  use  $\eta_c$  and  $J/\psi$  data/predictions to perform PDF fits from first principles

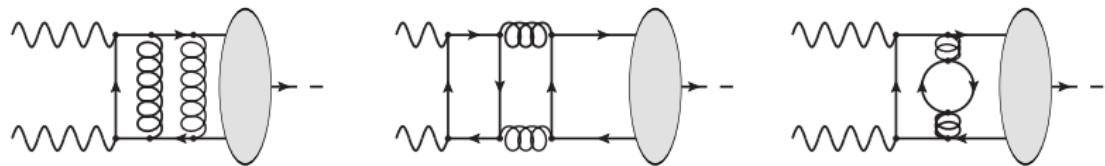
## Part II

# Two-loop master integrals and form-factors

# Form-factors

- compute two-loop form-factors analytically in different channels that contribute at NNLO accuracy
  - $\gamma\gamma \leftrightarrow \eta_Q \left(^1S_0^{[1]}\right) \rightarrow$  exclusive/inclusive decay
  - $gg \leftrightarrow \eta_Q \left(^1S_0^{[1]}\right) \rightarrow$  **hadro-production** and hadronic decay width
  - $\gamma g \leftrightarrow ^1S_0^{[8]} \rightarrow$  colour-octet contribution
  - $gg \leftrightarrow ^1S_0^{[8]} \rightarrow$  colour-octet contribution
  - $\gamma\gamma \leftrightarrow$  para-Positronium
- form-factors applicable to both production and decay
- in the past form-factors have been computed only in numerical form
  - $\eta_Q \rightarrow \gamma\gamma$  [A. Czarnecki, K. Melnikov, Phys.Lett.B 519 (2001) 212-218] [F. Feng, Y. Jia, W.-L. Sang, Phys.Rev.Lett. 115 (2015) 22, 222001]
  - para-Positronium  $\rightarrow \gamma\gamma$  [A. Czarnecki, K. Melnikov, A. Yelkhovsky, Phys.Rev.A 61 (2000) 052502]

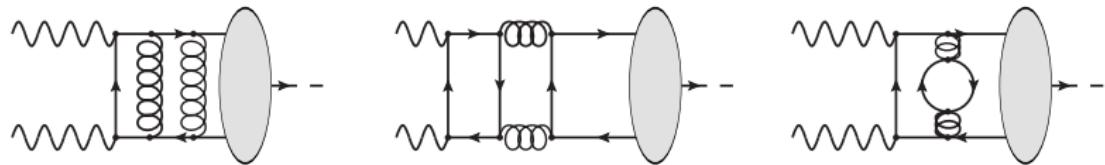
# Amplitude generation & partial fraction



$$\gamma(k_1)\gamma(k_2) \rightarrow Q(p_1)\bar{Q}(p_2) \quad (6)$$

- heavy quark momenta are equal  $p = p_1 = p_2$
- $k_1^2 = k_2^2 = 0$  for initial-state photons
- $p^2 = m_Q^2$  for final-state quarks
- threshold kinematics with  $\hat{s} = M_Q^2 = 4m_Q^2$  where  $M_Q = 2m_Q$

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- threshold kinematics with  $\hat{s} = M_Q^2 = 4m_Q^2$  where  $M_Q = 2m_Q$
- generate Feynman diagram with FeynArts ( $\sim 450$  diagrams for  $gg \leftrightarrow \eta_Q$  case)

# Graphical representation of Feynman integral

$$I_{\text{Coul.}} = \int d^D q \frac{1}{D_1 D_2 D_3 D_4} \text{ with}$$

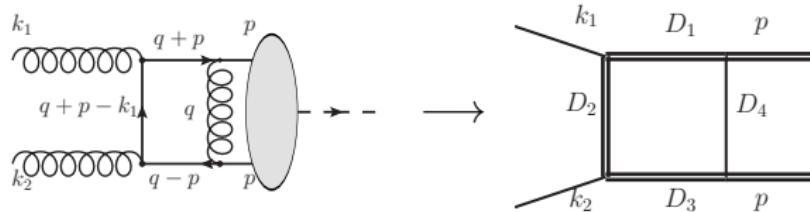
$$D_1 = (q + p)^2 - m_Q^2,$$

$$D_2 = (q + p - k_1)^2 - m_Q^2,$$

$$D_3 = (q - p)^2 - m_Q^2, \quad (7)$$

$$D_4 = q^2$$

- graphically represent Feynman integral similarly as Feynman diagram



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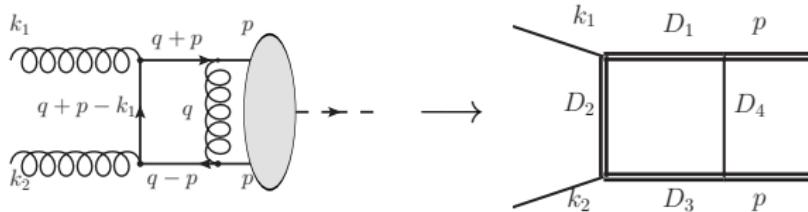
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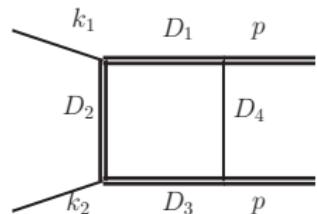
- graphically represent Feynman integral similarly as Feynman diagram



Rules: replace particles in Feynman diagram by simple lines

- single line  $\text{---}$  for massless ( $m = 0$ ) propagators/external legs
- double line  $\text{=====}$  for massive ( $m = m_Q$ ) propagators/external legs

# Graphical representation of Feynman integral



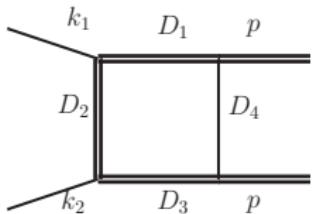
A Feynman diagram consisting of a rectangle divided into four quadrants by its diagonals. The top-left quadrant is labeled  $D_2$ , the top-right  $D_4$ , the bottom-left  $D_3$ , and the bottom-right  $D_1$ . External lines enter from the left at  $k_1$  and  $k_2$ , and exit at  $p$  from the top and right.

$$= \int d^D q \frac{1}{D_1 D_2 D_3 D_4}$$

such graphs

- incorporate **all** necessary information to define Feynman integral including propagators
- are **independent** of physics interaction (particles, coupling, QCD/QED/EW)
- satisfy at *each vertex* **momentum conservation**

# Graphical representation of Feynman integral



A Feynman diagram consisting of a square loop. The top horizontal edge is labeled  $D_1$  and  $p$ . The left vertical edge is labeled  $k_1$  and  $D_2$ . The bottom horizontal edge is labeled  $D_3$  and  $p$ . The right vertical edge is labeled  $k_2$  and  $D_4$ .

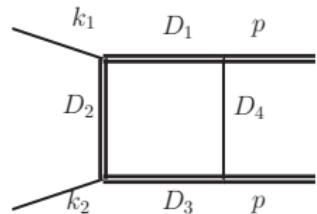
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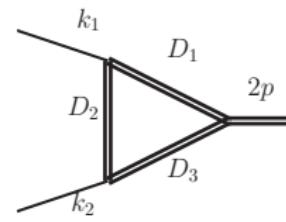
$$\int d^D q \frac{1}{D_1 D_2 D_3} = ?$$

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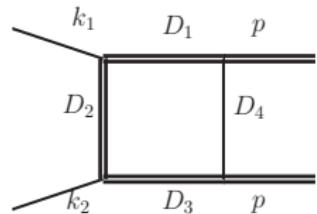

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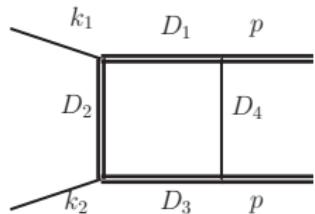
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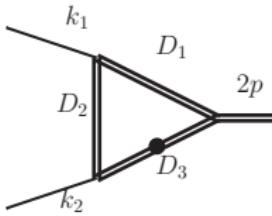
$$\int d^D q \frac{1}{D_1 D_2 D_3^2} = ?$$

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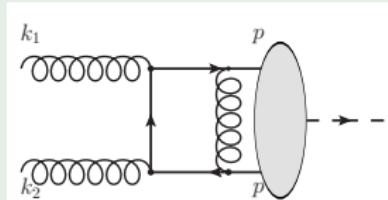
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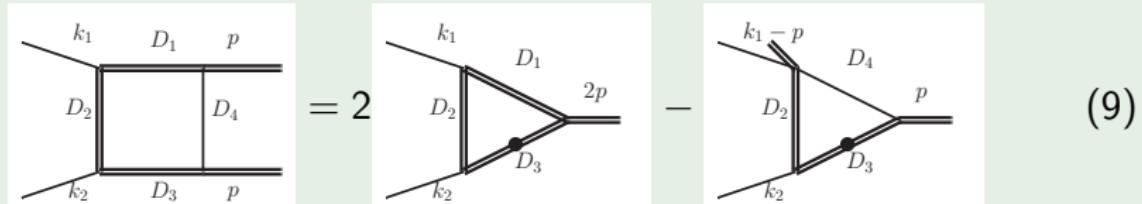
# Amplitude generation & partial fraction

## Example

Feynman diagram:



$$I_{\text{Coul.}} = \int d^D q \frac{1}{D_1 D_2 D_3 D_4} = \int d^D q \frac{2}{D_1 D_2 D_3^2} - \int d^D q \frac{1}{D_2 D_3^2 D_4} \quad (8)$$



# Topology and master integrals in a nutshell

- set of linearly independent denominators defines a Topology
  - # = all possible dot products of loop momentum  $\{q_1, q_2\}$  with itself and external momenta  $\{k_1, k_2\}$ 
    - $\rightarrow \{q_1^2, q_2^2, q_1 \cdot q_2, q_1 \cdot k_1, q_1 \cdot k_2, q_2 \cdot k_1, q_2 \cdot k_2\}$
    - $\rightarrow 7$  for our kinematics
  - each independent dot product can be described as linear combination of denominators  $\rightarrow$  tensor integral decomposition

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    - $\rightarrow 7$  for our kinematics
  - each independent dot product can be described as linear combination of denominators  $\rightarrow$  tensor integral decomposition
- Integration-By-Parts (IBP) technique: algebraic relations between Feynman integrals with different powers of denominators
  - large systems of relations
  - can reduce integrals with many denominators to integrals with few denominators  $\rightarrow$  **master integral**

# Amplitude

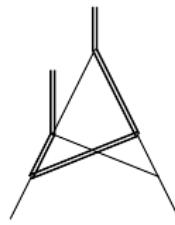
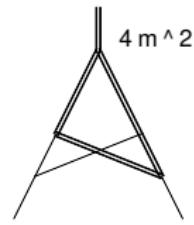
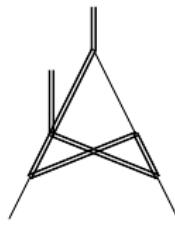
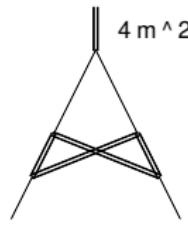
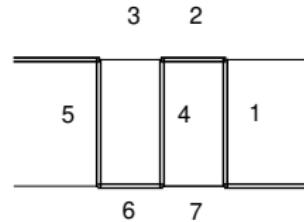
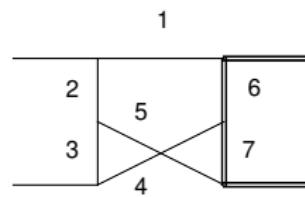
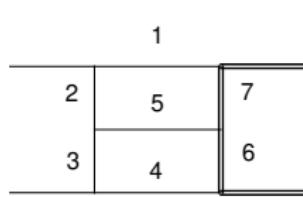
- two-loop Amplitude  $\mathcal{A}^{(2)}$ :

$$\mathcal{A}^{(2)} = \mathcal{A}^{(0)} \sum_{i=1}^{n_{\text{master}}} c_i(\epsilon) \text{MI}[i] \quad (10)$$

- tree-level Amplitude  $\mathcal{A}^{(0)}$
- coefficient  $c_i$  contains information on:
  - rational factor depending on dimensional regulator  $\epsilon$
  - colour factor ( $C_A, C_F, T_F$ )
  - number of massive ( $n_h$ ) and massless ( $n_l$ ) closed fermion loops  
(vacuum & light-by-light)
- need to compute master integrals  $\text{MI}[i]$

# Topologies and master integrals

Some examples of topologies:



# Topologies and master integrals

- Appearance of 77 master integrals
- These are seemingly independent, however we find some interesting equivalence relations among these

## Example

The diagram consists of two Feynman-like topologies connected by an equals sign (=). Both topologies have four external lines, each ending in a vertical bar. The left topology has a central node from which four internal lines extend to the four vertices where the external lines meet. The right topology has a similar structure but with a different internal line arrangement. To the right of the equals sign is the label (11).

(11)

- Analytical results for most of the integrals in these topologies are not available in the literature

## Direct Integration

Feynman integral can be represented via two graph polynomials  $\mathcal{U}$  and  $\mathcal{F}$  which are the first and second Symanzik polynomial respectively.

$$I = (-1)^a (e^{\epsilon \gamma_E})^h \Gamma\left(a - h \frac{D}{2}\right) \int_0^\infty dx_1 \dots \int_0^\infty dx_m \delta(1 - \Delta_H) \times \\ \times \prod_{i=1}^m \left( \frac{x_i^{a_i-1}}{\Gamma(a_i)} \right) \frac{\mathcal{U}^{a-(h+1)\frac{D}{2}}}{\mathcal{F}^{a-h\frac{D}{2}}} \quad (12)$$

## Direct Integration

Feynman integral can be represented via two graph polynomials  $\mathcal{U}$  and  $\mathcal{F}$  which are the first and second Symanzik polynomial respectively.

$$I = (-1)^a (e^{\epsilon \gamma_E})^h \Gamma\left(a - h \frac{D}{2}\right) \int_0^\infty dx_1 \dots \int_0^\infty dx_m \delta(1 - \Delta_H) \times \\ \times \prod_{i=1}^m \left( \frac{x_i^{a_i-1}}{\Gamma(a_i)} \right) \frac{\mathcal{U}^{a-(h+1)\frac{D}{2}}}{\mathcal{F}^{a-h\frac{D}{2}}} \quad (12)$$

- each  $x_i$  corresponds to a propagator ( $D_i \leftrightarrow x_i$ )
- $a_i$  is the power of denominator corresponding to  $x_i$
- $a = \sum a_i \rightarrow$  related to mass dimension of integral
- $\Delta_H$  is a linear combination of  $x_i$

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- $\Delta_H$  is a linear combination of  $x_i$ ;
- functions that will appear include *Multiple Polylogarithms* (MPLs) and *elliptic Multiple Polylogarithms* (eMPLs)

# Analytics and Numerics

- computed all integrals **analytically** via direct integration
- produced high-precision numerics (200 digits)
- validation of results numerically with pySecDec (only few digits)
- PSLQ procedure: allows to detect relations among complicated functions that appear  
→ can simplify to known/familiar functions (e.g.  $\log(2)$ ,  $\pi$ , etc.)

## Form-factors

Now ready to plug in analytics and numerics for the form-factors.

Validation of results,

- compare to known numerical results for  $\gamma\gamma \leftrightarrow \eta_Q$  case  
→ find full agreement [A. Czarnecki, K. Melnikov, Phys.Lett.B 519 (2001) 212-218] [F. Feng, Y. Jia, W.-L. Sang, Phys.Rev.Lett. 115 (2015) 22, 222001]
- for the new form-factors, validation is based on universal IR pole structure → amplitudes are manifestly finite after UV and IR renormalisation [Catani; Becher, Neubert]
- all amplitudes contain functions of maximal weight  $w = 4$  (e.g.  $\pi^4$ ,  $\log^4 2$ ,  $\pi\zeta_3$ ).
- regular Abelian corrections ( $C_F^2, C_F T_F n_{h/I}$ ) are identical for all form-factors → further confirmation of the new form-factor results
- QED corrections to para-Positronium result, agreement with existing numerical results in literature [A. Czarnecki, K. Melnikov, A. Yelkhovsky, Phys.Rev.A 61 (2000) 052502]

## Part III

# Decay of pseudo-scalar to di-photon at NNLO accuracy

## Exclusive decay width to di-photon

$$\Gamma_{\eta_Q \rightarrow \gamma\gamma} = \Gamma_0 \left[ 1 + \frac{\alpha_s}{\pi} \Gamma_1 + \left( \frac{\alpha_s}{\pi} \right)^2 \Gamma_{2,Q} \right] \quad (13)$$

$$\Gamma_1 = -3.3767985329702 \quad (14)$$

$$\Gamma_{2,c} = -65.288959657677 \quad (15)$$

$$- 7.5977966991830 \log \left( \frac{\mu_R^2}{m^2} \right) \quad (16)$$

$$\Gamma_{2,b} = -16.792206089919 \quad (17)$$

$$- 7.0349969436879 \log \left( \frac{\mu_R^2}{m^2} \right) \quad (18)$$

# Exclusive decay width to di-photon

- variation of scales
  - three scales in quarkonium physics:  $mv^2$ ,  $mv$ ,  $m$
  - $\mu_{\text{NRQCD}} = mv$ , ( $v^2 = 0.3$  for charmonium,  $v^2 = 0.1$  for bottomonium)
  - central:  $\mu_R = M = 2m$ , variation:  $\mu_R \in [M/\sqrt{2}, \sqrt{2}M]$

Charmonium:

$$\Gamma_{\eta_c \rightarrow \gamma\gamma}^{\text{NLO}} = \Gamma_0 \times [0.737^{+0.032}_{-0.044}] = (10.34^{+0.45}_{-0.62}) \text{ keV} \quad (19)$$

$$\boxed{\Gamma_{\eta_c \rightarrow \gamma\gamma}^{\text{NNLO}} = \Gamma_0 \times [0.28^{+0.11}_{-0.17}] = (3.9^{+1.6}_{-2.3}) \text{ keV}} \quad (20)$$

- $\mu_R$  uncertainty has contrary to expectation not reduced from NLO to NNLO
- latest experimental data [Particle Data Group]

$$\Gamma_{\eta_c \rightarrow \gamma\gamma}^{\text{exp}} = (5.06 \pm 0.34) \text{ keV} \quad (21)$$

- NNLO result is closer to experimental value than NLO result → importance of higher order corrections

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Bottomonium:

$$\Gamma_{\eta_b \rightarrow \gamma\gamma}^{\text{NLO}} = \Gamma_0 \times [0.809^{+0.016}_{-0.019}] = (3.977^{+0.077}_{-0.093}) \text{ keV} \quad (22)$$

$$\boxed{\Gamma_{\eta_b \rightarrow \gamma\gamma}^{\text{NNLO}} = \Gamma_0 \times [0.724^{+0.016}_{-0.018}] = (3.560^{+0.078}_{-0.087}) \text{ keV}} \quad (23)$$

- $\mu_R$  uncertainty is almost same for NLO and NNLO
- no experimental data available in [Particle Data Group]
- NNLO are important

# Summary

## Part I:

- a new scale prescription to cure the issue of negative cross-section and the mismatch between hard part and PDF
- PDFs are unconstrained at low scales → large PDF uncertainties for charmonium production

## Part II:

- two-loop double-virtual contributions involve massive Feynman integrals
- used cutting-edge techniques to compute all relevant master integrals analytically for the form-factor discussed and produced high-precision numerics

## Part III:

- shown that NNLO corrections to  $\eta_c$  decay to di-photon are large and turn out to be important as these are closer to experimental data than the NLO results
- however  $\mu_R$  uncertainties have contrary to expectation not reduced from NLO to NNLO (charmonium)

# Outlook

## Part I:

- application of new scale prescription to other charmonium states
- use charmonium data/predictions and constrain gluon PDFs through reweighting procedure

## Part II:

- application of techniques to master integrals with slightly different kinematics (off-shellness, additional gluon emission)

## Part III:

- computed two-loop form-factor ( $gg \rightarrow \eta_Q$ ) → now in a position to compute for the first time  $\eta_Q$  hadro-production up to NNLO accuracy in collinear/TMD factorisation

# Thanks for attention!