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Quarkonium production in MadGraph5_aMC@NLO

Quarkonia as Tools 2025

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January 8, 2025

- 1 Introduction
- 2 MadGraph5: onium implementation
- 3 TMD factorisation and TMDs
- 4 Conclusions

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MadGraph5_aMC@NLO = event / diagram generator (Python)
↪ compute matrix-element (helicity amplitude formalism)



- Total cross section
- Differential cross section
- Un-weighted event



Master integral for symmetric collisions in MadGraph5:

$$\sigma(AA \rightarrow X) = \sum_{i,j} \int dx_i dx_j d\Phi f_{i/A}(x_i) f_{j/A}(x_j) \hat{\sigma}_{(ab \rightarrow X)}(x_i, x_j, \mu_F, \mu_R)$$

How MadGraph5 works:

- Identify partonic processes and calculate **partonic cross section**
- Use **PDFs (LHAPDF package)**
- Do **phase space integral** and convolute with **PDFs**
- Generate events

NEW implementations:

- Asymmetric collisions [see Carlo's talk]
- **Quarkonium production!** (this talk)

There are many reasons why quarkonia are interesting:

- QCD studies!
- internal structure of nucleons
- gluon investigation (e.g. EIC)
- ...

→ TMDs!!

Focus on inclusive processes → factorisation:

$$\sigma(pp \rightarrow Q + X) = \sum_{i,j,n} \int dx_1 dx_2 f_{i/p}(x_1) f_{j/p}(x_2) \times \hat{\sigma}(ij \rightarrow Q\bar{Q}[n] + X) \langle \mathcal{O}_n^Q \rangle \quad \boxed{n = 2s+1 \quad L_J^C}$$

Models for quarkonium production: NRQCD, CSM, CEM, ...

Motivation: why automation of quarkonium cross sections?

Many reasons, including:

- global data-theory comparisons
- physics cases for future experimental facilities
- global NRQCD fits

Matrix element/event generators publicly available

(↔ interfacing of e.g. HERWIG or PYTHIA with e.g. MG5_aMC)



facilitates complete computation

- ✓ versatility and enhanced physics simulation capabilities
- ✗ integration complexity, computational overhead, code compatibility and increased learning requirements

MadOnia:

- ✓ single quarkonium production phenomenology (only)
- ✗ (deprecated) module within MadGraph4

Helac-Onia:

- ✓ (S-wave/P-wave) multiple-quarkonium production based on tree-level helicity amplitudes
- ✗ limited to LO (not immediately extendable to NLO)

MadGraph5_aMC@NLO:

- ✓ flexibility to support SM, BSM and large number of particle physics models
- ? no quarkonia final states → (technical) complexities arise!

Goal: automation of **LO quarkonium** with NLO in sight

- 1 Introduction
- 2 MadGraph5: onium implementation**
- 3 TMD factorisation and TMDs
- 4 Conclusions

- Implementation of quarkonia in MadGraph5_aMC@NLO at LO
 - ↪ Single and multiple S-wave inclusive quarkonium production
 - Colour projectors
 - Spin projectors
 - Interface
 - Phase space adaptation

- Extensions to states with leading P-wave Fock states
LO implementation → □ NLO in the easiest way possible!

- TMD factorisation also to be implemented
 - ↪ for example $gg \rightarrow di\text{-}J/\psi$ (... not only for quarkonia)

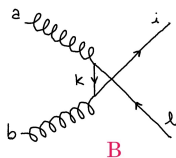
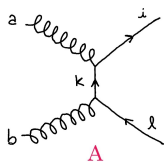
- Implementation of quarkonia in MadGraph5_aMC@NLO at LO
 - ↪ Single and multiple S-wave inclusive quarkonium production
 - Colour projectors → implemented ✓
 - Spin projectors → implemented ✓
 - Interface → implemented ✓
 - Phase space adaptation
- Extensions to states with leading P-wave Fock states
LO implementation → □ NLO in the easiest way possible!
- TMD factorisation also to be implemented
 - ↪ for example $gg \rightarrow di-J/\psi$

Quarkonium in the quantum state $n \rightarrow$ colour singlet or octet?

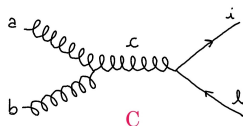
$$\mathbb{P}_1 = \delta_{ij} / \sqrt{N_c}$$

$$\mathbb{P}_8 = \sqrt{2} t_{ij}^c$$

- Example: $gg \rightarrow c\bar{c}$ 3 diagrams at LO

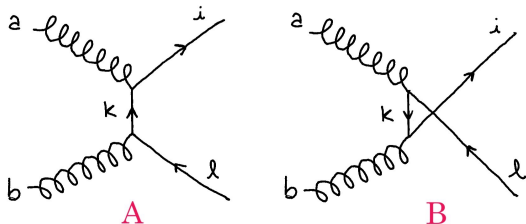


Colour Singlet contribution



Colour Octet contribution

Colour projectors \mathbb{P}_C (2)

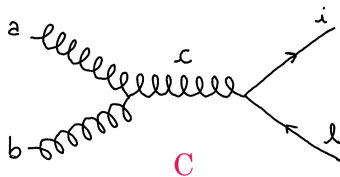


$$(A) \sim (t_{ik}^a t_{kl}^b) = (t^a t^b)_{il} \quad \rightarrow \text{we set } (t^a t^b)_{il} = c_1$$

$$(B) \sim (t_{ik}^b t_{kl}^a) = (t^b t^a)_{il} \quad \rightarrow \text{we set } (t^b t^a)_{il} = c_2$$

\hookrightarrow open $c\bar{c}$ colour basis of $\dim = 2$

Colour projectors \mathbb{P}_C (3)



$$\begin{aligned}
 (\mathbf{C}) &\sim f^{abc}(t_{ij}^c) = (t^a t^b)_{ij} - (t^b t^a)_{ij} \\
 &= c1 - c2
 \end{aligned}$$

$$c1c1^\dagger = (t^a t^b)_{ij}(t^b t^a)_{ij} = \text{Tr}(t^a t^b t^b t^a) = \frac{16}{3}$$

⋮

$$\longrightarrow \text{colour matrix: } \begin{pmatrix} c1c1^\dagger & c1c2^\dagger \\ c2c1^\dagger & c2c2^\dagger \end{pmatrix}$$

Apply colour projectors: $\mathbb{P}_1 = \delta^{il}$ and $\mathbb{P}_8 = t_{ij}^c$

- Colour singlet:

$$(t^a t^b)_{il} \delta^{il} = \text{Tr}(t^a t^b) \quad (\text{A})$$

$$(t^b t^a)_{il} \delta^{il} = \text{Tr}(t^b t^a) \quad (\text{B})$$

- Colour octet:

$$\left. \begin{aligned} (t^a t^b)_{il} t_{ij}^c &= \text{Tr}(t^a t^b t^c) = \frac{1}{4}(d^{abc} + if^{abc}) & (1) \\ (t^b t^a)_{il} t_{ij}^c &= \text{Tr}(t^b t^a t^c) = \frac{1}{4}(d^{bac} + if^{bac}) & (2) \end{aligned} \right\} (1) - (2): \quad (\text{C})$$

The amplitude will be given by the sum of the three contributions

$$\mathcal{A} = A(\text{A}) + A(\text{B}) + A(\text{C})$$

Colour projectors for m colour singlet and colour octet quarkonia production and associated production implemented ✓

Metacode: quarkonium formalism implemented via extension of python files which produce fortran code → numerical manipulations

In `/mg5amcnlo/madgraph/core`

- `color_algebra.py`
- `color_amp.py`
- `helas_objects.py`

Quarkonium in the quantum state $n \rightarrow$ spin singlet or triplet?

- Considering $a(k_1)b(k_2) \rightarrow Q(k_3)\bar{Q}(k_4)$: JHEP 07 (2024), 050

$$\mathcal{A}(r) = \bar{u}_{\lambda_Q}(k_3)\Gamma(r)v_{\lambda_{\bar{Q}}}(k_4)$$

- Apply colour projector: $\mathcal{A}_{\{C\}}(r) = \sum_{c_3, c_4} \mathbb{P}_C \mathcal{A}(r)$
- Apply spin projector: $\mathcal{A}_{\{C, S\}}(r) = \sum_{\lambda_Q, \lambda_{\bar{Q}}} \mathbb{P}_S \mathcal{A}_{\{C\}}(r)$

$$\mathbb{P}_S = \frac{\bar{v}_{\lambda_{\bar{Q}}}(k_4)\Gamma_S u_{\lambda_Q}(k_3)}{2\sqrt{2m_Q m_{\bar{Q}}}} \quad S = 0, \Gamma_S = \gamma_5; 1, \Gamma_S = \not{K}$$

Declaration of new effective spinors in:

- `/mg5amcnlo/aloha/template_files/aloha_functions.f`
- `/mg5amcnlo/madgraph/core/helas_objects.py`

Python: calls `template_files` \rightarrow `matrix_i.f` files

Amplitudes organised into colour basis JAMPs

$$\mathcal{A} = \sum_i A_i \stackrel{\text{example}}{=} A(\mathbf{A}) + A(\mathbf{B}) + A(\mathbf{C})$$

$$A(\mathbf{A}) = c_1 A_1 \quad A(\mathbf{B}) = c_2 A_2 \quad A(\mathbf{C}) = c_1 A_{31} - c_2 A_{32}$$

$$\underline{\text{JAMP decomposition}} \quad \begin{cases} \text{JAMP}_1 & = A_1 + A_{31} \propto c_1 \\ \text{JAMP}_2 & = A_2 - A_{32} \propto c_2 \end{cases}$$

$$|\mathcal{A}|^2 = \sum_{i,j=1,2} \text{JAMP}_i^* \langle c_i | c_j \rangle \text{JAMP}_j$$

(Depends on spin projectors - constructed from helas routines)

Efficiency: large number of Feynman diagrams possible...

...but **colour basis much smaller!**

Generate process: single, associated and multiple production

From the mg5amcnlo folder: type `./bin/mg5_aMC`

MG_aMC >

★ Example: $pp \rightarrow J/\psi + c\bar{c}g$

MG_aMC > generate p p > `c.c~(1|3S11)` c c~ g

MG_aMC > generate p p > `c.c~(1|3S18)` c c~ g

dot notation for onia with spectroscopic notation in brackets

or

MG_aMC > generate p p > `jpsi` c c~ g

Particle name directly in the process generation

New files containing onium information in the input folder:

- `boundstates_default.txt`
- `fockstates_default.txt`

Interface implementation made in `/madgraph/interface/`

```

#
# Quarkonium Boundstates (S-waves only)
#
# Syntax: label = Fock states (separated by spaces)
#
# Charmonium
etac = c.c~(1|1S01) c.c~(1|1S08)
etac(2s) = c.c~(2|1S01) c.c~(2|1S08)
jpsi = c.c~(1|3S11) c.c~(1|3S18)
psi(2s) = c.c~(2|3S11) c.c~(2|3S18)
# Charmed B mesons
bc+ = c.b~(1|1S01) c.b~(1|1S08)
b*c+ = c.b~(1|3S11) c.b~(1|3S18)
bc- = b.c~(1|1S01) b.c~(1|1S08)
b*c- = b.c~(1|3S11) b.c~(1|3S18)
# Bottomonium
etab = b.b~(1|1S01) b.b~(1|1S08)
etab(2s) = b.b~(2|1S01) b.b~(2|1S08)
upsilon = b.b~(1|3S11) b.b~(1|3S18)
upsilon(2s) = b.b~(2|3S11) b.b~(2|3S18)
# Toponium
etat = t.t~(1|1S01) t.t~(1|1S08)
etat(2s) = t.t~(2|1S01) t.t~(2|1S08)

```

```
# N: principal quantum number
# S: spin type
# L: orbital angular momentum quantum number
# J: total angular momentum quantum number
# C: color type
```

pid	pythia	name	notation	particle	anti-particle	N	S	L	J	C	charge
#####											
# Charmonia #											
#####											
# etac											
4411001	441	etac(1 1S01)	c.c~(1 1S01)	c	c~	1	1	0	0	1	0
4411008	9940001	etac(1 1S08)	c.c~(1 1S08)	c	c~	1	1	0	0	8	0
4421001	100441	etac(2 1S01)	c.c~(2 1S01)	c	c~	2	1	0	0	1	0
4421008	9999999	etac(2 1S08)	c.c~(2 1S08)	c	c~	2	1	0	0	8	0
# J/psi											
4413011	443	jpsi(1 3S11)	c.c~(1 3S11)	c	c~	1	3	0	1	1	0
4413018	9940003	jpsi(1 3S18)	c.c~(1 3S18)	c	c~	1	3	0	1	8	0
4423011	100443	psi(2 3S11)	c.c~(2 3S11)	c	c~	2	3	0	1	1	0
4423018	9940103	psi(2 3S18)	c.c~(2 3S18)	c	c~	2	3	0	1	8	0
#####											
# Charmed B mesons #											
#####											
# Meson											
5411001	541	bc+(1 1S01)	c.b~(1 1S01)	c	b~	1	1	0	0	1	1
5411008	9999999	bc+(1 1S08)	c.b~(1 1S08)	c	b~	1	1	0	0	8	1
5413011	543	b*c+(1 3S11)	c.b~(1 3S11)	c	b~	1	3	0	1	1	1
5413018	9999999	b*c+(1 3S18)	c.b~(1 3S18)	c	b~	1	3	0	1	8	1

```
MG5_aMC>display boundstates
Bound state labels:
etac = c.c~(1|1S01) c.c~(1|1S08)
etac(2s) = c.c~(2|1S01) c.c~(2|1S08)
jpsi = c.c~(1|3S11) c.c~(1|3S18)
psi(2s) = c.c~(2|3S11) c.c~(2|3S18)
bc+ = c.b~(1|1S01) c.b~(1|1S08)
b*c+ = c.b~(1|3S11) c.b~(1|3S18)
bc- = b.c~(1|1S01) b.c~(1|1S08)
b*c- = b.c~(1|3S11) b.c~(1|3S18)
etab = b.b~(1|1S01) b.b~(1|1S08)
etab(2s) = b.b~(2|1S01) b.b~(2|1S08)
epsilon = b.b~(1|3S11) b.b~(1|3S18)
epsilon(2s) = b.b~(2|3S11) b.b~(2|3S18)
etat = t.t~(1|1S01) t.t~(1|1S08)
etat(2s) = t.t~(2|1S01) t.t~(2|1S08)
```

```
MG5_aMC>generate g g > jpsi g
INFO: Trying to generate process g g > c.c~(113S11) g
INFO: Checking for minimal orders which gives processes.
INFO: Please specify coupling orders to bypass this step.
INFO: Trying coupling order WEIGHTED<=3: WEIGHED IS QCD+2*QED
INFO: Trying process: g g > c c~ g WEIGHTED<=3 @1
INFO: Process has 16 diagrams
1 processes with 16 diagrams generated in 0.029 s
Total: 1 processes with 16 diagrams
INFO: Trying to generate process g g > c.c~(113S18) g
INFO: Checking for minimal orders which gives processes.
INFO: Please specify coupling orders to bypass this step.
INFO: Trying coupling order WEIGHTED<=3: WEIGHED IS QCD+2*QED
INFO: Trying process: g g > c c~ g WEIGHTED<=3 @1
INFO: Process has 16 diagrams
1 processes with 16 diagrams generated in 0.029 s
Total: 2 processes with 32 diagrams
```

Partial list of processes that have been checked (49 up to now):

- `g g > c.c~(1|1S01)`
- `g g > b.b~(1|1S08)` `single`
- `g g > b.b~(1|1S01) g` `single + elem.part.`
- `g g > b.b~(1|1S01) b.b~(1|1S01)`
- `g g > b.b~(1|1S01) c.c~(1|1S01)` `multiple`

Benchmarked our matrix elements squared against Helac-Onia:



- $g g \rightarrow b \bar{b} (1 | 1S01) g$

Phase-space point			
E	px	py	pz
0.5000000E+03	0.0000000E+00	0.0000000E+00	0.5000000E+03
0.5000000E+03	0.0000000E+00	0.0000000E+00	-0.5000000E+03
0.5000048E+03	0.1109232E+03	0.4448265E+03	-0.1995510E+03
0.4999952E+03	-0.1109232E+03	-0.4448265E+03	0.1995510E+03

Matrix element	1.4532913707599472E-005 GeV ⁰
Helac-Onia	1.45329122E-05 GeV ⁰
Ratio	1.0000001005670054

- $g g > b.\bar{b}(1|3S11) g$

Matrix element	4.8065942918292797E-010 GeV ⁰
Helac-Onia	4.80663009E-10 GeV ⁰
Ratio	0.99999255151418964

- $g g > c.\bar{c}(1|1S01) g$

Matrix element	4.4080653118388797E-005 GeV ⁰
Helac-Onia	4.40806543E-05 GeV ⁰
Ratio	0.99999997242730454

- $g g > b.\bar{b}(1|1S01) b.\bar{b}(1|1S01)$

Matrix element	5.2953309332877083E-013 GeV ⁰
Helac-Onia	5.29533448E-13 GeV ⁰
Ratio	0.99999932957700877

Phase space integration in MadGraph5: **multi-channelling**
↔ efficiency: parallel computation

Phase-space adaptation: onia in final state **single** particle, not two!

- Process like $gg \rightarrow c\bar{c}$ always interpreted as $2 \rightarrow 2$ process

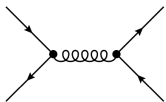
How to perform phase-space integration for onia in MG5:

- VEGAS algorithm (already in MG5)
- Single-diagram-enhanced multi-channel integration
- **Application to quarkonium production**

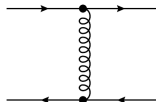
↔ new parameterisation required!
(ex. two t-channel peaks: issue with integration...)

slide courtesy of L. Simon

Example: $q\bar{q} \rightarrow q\bar{q}$



peak in s



peak in t

Single-diagram-enhanced multi-channel integration [Maltoni, Stegler (2003)]:

$$\int d\Pi_2 |\mathcal{A}_1 + \mathcal{A}_2|^2 = \int d\Pi_2 \left(\underbrace{|\mathcal{A}_1|^2 \frac{|\mathcal{A}_1 + \mathcal{A}_2|^2}{|\mathcal{A}_1|^2 + |\mathcal{A}_2|^2}}_{\text{peak in } s} + \underbrace{|\mathcal{A}_2|^2 \frac{|\mathcal{A}_1 + \mathcal{A}_2|^2}{|\mathcal{A}_1|^2 + |\mathcal{A}_2|^2}}_{\text{peak in } t} \right)$$

Phase-space parametrisation [Byckling, Kajantie (1971)]:

$$\int d\Pi_n \sim \int dM_{n-1} \int d\Omega_n \cdots \int dM_2 \int d\Omega_3 \int d\Omega_2$$

$$\int d\Pi_n \sim \int dM_{n-1} \int d\phi_n \int dt_{n-1} \cdots \int dM_2 \int d\phi_3 \int dt_2 \int d\phi_2 \int dt_1$$



New parts in the code: search
ONIA

GitHub: release **onia** branch of MG5
version 3.x

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[see Nanako's talk]

Understanding the internal structure of the nucleon \rightarrow TMDsCorrelations between k_T and the polarisation of the nucleon/parton2 components \triangleright collinear (x) \triangleright transversal (\vec{k}_\perp) \rightarrow generate q_T (final-state)**TMD factorisation** ($q_T \ll Q$ hard scale)

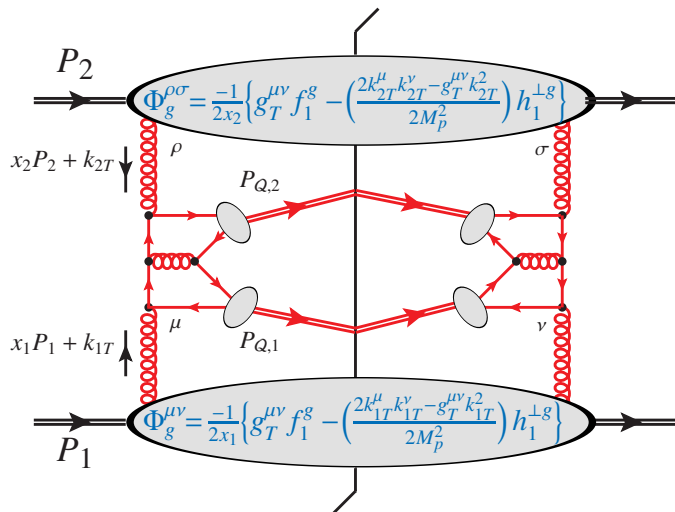
General factorised cross section

 \hookrightarrow partonic scattering amplitude (*perturbative*) \hookrightarrow k_T -dependent correlators (*non-perturbative*)

$$d\sigma = \int dx_1 dx_2 d^2\vec{k}_{T1} d^2\vec{k}_{T2} \delta^{(2)}(\vec{k}_{T1} + \vec{k}_{T2} - \vec{q}_T) \\ \times \Phi_g^{\mu\nu}(x_1, \vec{k}_{T1}) \Phi_g^{\rho\sigma}(x_2, \vec{k}_{T2}) \left[\hat{M}_{\mu\rho} \hat{M}_{\nu\sigma}^* \right]_{\substack{k_1=x_1 P_1 \\ k_2=x_2 P_2}} + \mathcal{O}\left(\frac{q_T^2}{Q^2}\right)$$

LO Feynman diagram for $p(P_1) + p(P_2) \rightarrow Q(P_{Q,1}) + Q(P_{Q,1}) + X$

F. Scarpa, D. Boer, M.G. Echevarria, J.-P. Lansberg, M. Schlegel, EPJC (2020) 80:87



[see Nanako's talk]

J.-P. Lansberg, C. Pisano, F. Scarpa, M. Schlegel, PLB 784(2018) 217

The general formula for the cross section of gluon fusion is:

$$\begin{aligned}
 d\sigma^{gg} \propto & F_1 \times \mathcal{C}[f_1^g f_1^g] \\
 & + F_2 \times \mathcal{C}[w_2 h_1^{\perp g} h_1^{\perp g}] \\
 & + (F_3 \times \mathcal{C}[w_3 f_1^g h_1^{\perp g}] + F'_3 \times \mathcal{C}[w'_3 h_1^{\perp g} f_1^g]) \cos(2\Phi_{CS}) \\
 & + (F_4 \times \mathcal{C}[w_4 h_1^{\perp g} h_1^{\perp g}]) \cos(4\Phi_{CS})
 \end{aligned}$$

- F_i : hard scattering coefficients
- w_j : transverse weights
- f_1^g and $h_1^{\perp g}$: unpolarised and linearly polarised gluon TMDs
- Φ_{CS} : Collins-Soper azimuthal angle

$$\begin{aligned} \rightarrow d\sigma = & \frac{(2\pi)^4}{S^2} dPS_n \sum_{\lambda_a, \bar{\lambda}_a, \lambda_b, \bar{\lambda}_b = \pm 1} \frac{1}{(N_c^2 - 1)^2} \times \\ & \sum_{a, b; l} \mathcal{A}_{\lambda_a, \lambda_b; l}^{ab}(\bar{k}_a, \bar{k}_b; \{P_i\}) \mathcal{A}_{\bar{\lambda}_a, \bar{\lambda}_b; l}^{ab*}(\bar{k}_a, \bar{k}_b; \{P_i\}) \times \\ & \int d^2 k_{aT} \int d^2 k_{bT} \delta^{(2)}(d^2 k_{aT} + d^2 k_{bT} - d^2 q_T) \times \\ & \Phi_{\bar{\lambda}_a, \lambda_a}(x_a, d^2 k_{aT}, \zeta_a, \mu) \Phi_{\bar{\lambda}_b, \lambda_b}(x_b, d^2 k_{bT}, \zeta_b, \mu) + \mathcal{O}(q_T/Q) \end{aligned}$$

$$\Phi_{\lambda_a, \bar{\lambda}_a} = \frac{1}{2x_a} \left(\delta_{\lambda_a, \bar{\lambda}_a} f_1^g + \frac{k_{ax}^2 - k_{ay}^2 - 2i\lambda_a k_{ax} k_{ay}}{2M^2} \delta_{\lambda_a, -\bar{\lambda}_a} h_1^{\perp g} \right)$$

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Implementation of quarkonia in MG5: in progress!

- ★ **Colour projectors** implemented
- ★ **Spin-projectors** implemented
- ★ **Interface** implemented
- ★ **Benchmarked our matrix elements squared against Helac-Onia**
- **Phase-space adaptation** in progress!
- Application: $J/\psi + H$ hadroproduction arXiv:2109.02025

outlook

- **P-wave** extension
- From LO to **NLO!** arXiv:2402.19221
- **TMD factorisation**

Backup slides

(1) Phase-space integration: VEGAS algorithm

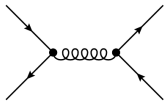
slide courtesy of L. Simon

Approximation of probability distribution [\[edit\]](#)

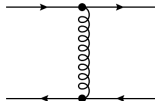
The VEGAS algorithm approximates the exact distribution by making a number of passes over the integration region while [histogramming](#) the function f . Each histogram is used to define a sampling distribution for the next pass. Asymptotically this procedure converges to the desired distribution. In order to avoid the number of histogram bins growing like K^d with dimension d the probability distribution is approximated by a separable function: $g(x_1, x_2, \dots) = g_1(x_1)g_2(x_2) \dots$ so that the number of bins required is only Kd . [This is equivalent to locating the peaks of the function from the projections of the integrand onto the coordinate axes.](#) The efficiency of VEGAS depends on the validity of this assumption. It is most efficient when the peaks of the integrand are well-localized. If an integrand can be rewritten in a form which is approximately separable this will increase the efficiency of integration with VEGAS.

[\[wikipedia\]](#)

Example: $q\bar{q} \rightarrow q\bar{q}$



peak in s



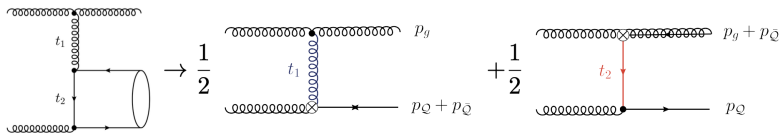
peak in t

[Diagrams drawn with FeynGame]

(2) Phase-space integration: quarkonium production

slide courtesy of L. Simon

Example: $gg \rightarrow Q\bar{Q}[n]g$



Issue: Two t -channel peaks, but only one can be integration parameter

$$\text{either } \int d\Pi_2 \sim \int dt_1 \quad \text{or} \quad \int d\Pi_2 \sim \int dt_2$$

Solution:

$$\int d\Pi_2 = \frac{1}{2} \int \underbrace{d\Pi_2}_{\sim dt_1} + \frac{1}{2} \int \underbrace{d\Pi_2}_{\sim dt_2}$$

- ▶ Momentum $p_Q + p_{\bar{Q}}$ of bound state is integration parameter
- ▶ Momentum p_Q of bound state's parton is integration parameter
→ new parametrisation is required

