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Extensions of MadGraph5_aMC@NLO for bound-state production studies

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I present the first implementation in MadGraph5_aMC@NLO of leading-order (LO) cross sections for S-wave quarkonium, leptonium and B_c-meson bound-state production in Non-Relativistic QCD and Non-Relativistic QED. In these proceedings, I specifically report on the extension of MadGraph5_aMC@NLO to quarkonium states, the simplest bound states in QCD, and describe the capabilities of our new tool for quarkonium production in a wide variety of collider environments. I present a comprehensive benchmarking of our LO tool against Helac-Onia, followed by a demonstration of its expanded capabilities, enabling studies complementing and extending state-of-the-art phenomenology. This work provides the community with an all-encompassing tool for quarkonium-production studies in QCD, delivering reliable, efficient and fast automated computations and lays the foundation for our future NLO extensions.

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1. Introduction

MadGraph5_aMC@NLO (MG5) [1] is a Monte-Carlo (MC) event-generator dedicated to the computation of (differential) cross sections and particle-event generation, through a fully-automated workflow seamlessly integrating Feynman-diagram generation from a given Lagrangian in Quantum Field Theory, their amplitude construction based on a given set of Feynman rules, and finally cross sections in a variety of formats, including the universal Les Houches Event (LHE) standard. It aims at providing all the elements needed for Standard Model (and beyond) phenomenology. The master integral within the collinear-factorisation formalism, used in the computations for an inclusive process, is

$$\mathrm{d}\sigma(h_A+h_B \to k+X) = \sum_{a,b} \int \mathrm{d}x_a \mathrm{d}x_b f_{a/h_A}(x_a) f_{b/h_B}(x_b) \mathrm{d}\hat{\sigma}(ab \to k+X)(x_a, x_b, \mu_F, \mu_R), \quad (1)$$

where $h_{A,B}$ are the hadrons in the initial state, k is the considered final-state elementary particle(s), a and b are the partons coming from the two initial hadrons, $x_{a,b}$ are the momentum fraction carried by each of them, $f_{a/h_A}(x_a)$ and $f_{b/h_B}(x_b)$ are the Parton Distribution Functions and $\mathrm{d}\hat{\sigma}(ab \to k+X)$ is the partonic cross section, which depends on parton momenta, factorisation (μ_F) and renormalisation (μ_R) scales. Importantly, *bound-state* production of elementary particles is not supported. In this work, we extend the capability of MG5 in this direction, including quarkonium, leptonium and charmed B-meson production, at the Leading Order (LO) for S-wave particle states. In these proceedings, we report on quarkonium production only, while a complete discussion, including B_c and leptonium production, implemented in a MC for the first time, is available in [2].

2. Overview of quarkonium production in NRQCD

Composite particles made of a heavy quark and its correspondent antiquark, known as quarkonia, represent the simplest bound states in Quantum Chromo-Dynamics (QCD). They serve as the perfect playground for QCD studies, from both a theoretical and an experimental point of view [3]. Quarkonium production can be described following the Non-Relativistic QCD (NRQCD) [4] formalism: considering an inclusive process $h_A + h_B \to \mathcal{Q} + X$, where the two hadrons h_A, h_B generate a quarkonium $\mathcal{Q}$ in the final state, the cross section in eq. (1) can be further factorised as

$$\mathrm{d}\sigma(h_A + h_B \to \mathcal{Q} + X) = \sum_{a,b,n} \int \mathrm{d}x_a \mathrm{d}x_b f_{a/h_A}(x_a) f_{b/h_B}(x_b) \mathrm{d}\hat{\sigma}(ab \to Q\bar{Q}[n] + X) \langle \mathcal{O}_n^{\mathcal{Q}} \rangle, \quad (2)$$

with $Q\bar{Q}[n]$ the open heavy quark and antiquark pair, in the state n defined as

$$n = {}^{2S+1}L_J^{[C]}, \quad (3)$$

using the spectroscopic notation. $\langle \mathcal{O}_n^{\mathcal{Q}} \rangle$ represents the quarkonium bound state parametrised by Long-Distance Matrix Elements (LDMEs), which encode the probability of the heavy-quark pair to evolve into the bound state. The quantum numbers in eq. (3) are S for the spin, L for the orbital angular momentum, J for the total angular momentum and C for the colour: we consider in the following either spin-singlet or spin-triplet states ($2S + 1 = 1$ or 3 respectively), and either colour-singlet or colour-octet states ($C = 1$ or 8). The amplitude for a $2 \to N$ process, that we refer to as r, can be expressed as [5, 6]

$$\mathcal{A}^{(N)}(r) = \bar{u}_{\lambda_Q}(k_Q)\Gamma(r)v_{\lambda_{\bar{Q}}}(k_{\bar{Q}})\,, \tag{4}$$

where $\bar{u}, v$ are the heavy-quark and antiquark Dirac spinors, $\lambda_Q, \lambda_{\bar{Q}}$ their helicities, $k_Q, k_{\bar{Q}}$ their momenta and $\Gamma(r)$ the amputated amplitude encoding the Dirac algebra. Calling $c_Q, c_{\bar{Q}}$ the colour indices of the heavy quark and the antiquark, the colour-projected amplitude can be written as

$$\mathcal{A}^{(N)}_{\{C\}}(r) = \sum_{c_Q, c_{\bar{Q}}} \mathbb{P}_C \mathcal{A}^{(N)}(r)\,, \tag{5}$$

where $\mathbb{P}_C$ is the colour projector, either of the form $\mathbb{P}_C = \delta_{c_Q c_{\bar{Q}}}/\sqrt{N_c}$ for a colour-singlet or $\mathbb{P}_C = \sqrt{2}T^{c_Q\bar{Q}}_{c_{\bar{Q}}c_Q}$ for a colour-octet Fock state, with $T^{c_Q\bar{Q}}_{c_{\bar{Q}}c_Q}$ the Gell-Mann matrix. Following a similar reasoning, the spin-projected amplitude can be written as

$$\mathcal{A}^{(N)}_{\{C,S\}}(r) = \sum_{\lambda_Q, \lambda_{\bar{Q}}} \mathbb{P}_S \mathcal{A}^{(N)}_{\{C\}}(r)\,, \tag{6}$$

where $\mathbb{P}_S$ is the spin projector, defined as

$$\mathbb{P}_S = \frac{\bar{v}_{\lambda_{\bar{Q}}}(k_{\bar{Q}})\Gamma_S\, u_{\lambda_Q}(k_Q)}{2\sqrt{2m_Q m_{\bar{Q}}}}\,, \tag{7}$$

with $m_Q, m_{\bar{Q}}$ the mass of the heavy quark and antiquark, and $\Gamma_S = \gamma_5$ for a spin-singlet quarkonium or $\Gamma_S = \not{\varepsilon}^*_{\lambda_S}(K)$ for a spin-triplet quarkonium. In the latter case, $\not{\varepsilon}^* = \varepsilon^{*\mu}\gamma_\mu$, involving the polarisation vector of the quarkonium, which depends on the total momentum of the heavy-quark pair, K, and $\lambda_S = 0, \pm 1$ labelling the polarisation components of the S orbital-angular-momentum state. After projection, Q and $\bar{Q}$ combine into an effective particle in the quantum state n defined in eq. (3), and the amplitude of the resulting process $\dot{r}$ can be written as

$$\mathbb{A}^{(N-1)}(\dot{r}) = \mathcal{A}^{(N)}_{\{C,S\}}(r), \tag{8}$$

which is related to the differential partonic cross section as

$$\mathrm{d}\hat{\sigma} \propto \sum_{\substack{\text{colour}\\ \text{spin}}} |\mathbb{A}^{(N-1)}(\dot{r})|^2\, \mathrm{d}\phi_{N-1}(\dot{r})\,. \tag{9}$$

Here $\mathrm{d}\phi_{N-1}(\dot{r})$ represents the phase-space element of the $(N-1)$-body phase space, and so the integration over it is performed after combining the two heavy quarks into the quarkonium state.

3. Implementation

Quarkonium bound states are a superposition of different Fock states. In `MG5` they are now defined similarly to `multiparticles`, for example the J/ψ is defined as

```
Jpsi = Jpsi(1|3S11) Jpsi(1|1S08) Jpsi(1|3S18)
```

where `Jpsi` is the physical bound state and the single Fock states are defined with the name of the particle (`Jpsi` here) and the spectroscopic notation in round brackets: the first number is the principal quantum number (1 for the ground state), following on the right there is $2S + 1$ (1 or 3), L, which in the current implementation is $L = 0$ (S) then J and the colour C as the last digit (1 or 8). The user can display all the bound states directly from the interface in `MG5`, opening it from the terminal in the `mg5amcnlo` with `./bin/mg5_aMC` and typing the command `display boundstates`. We have implemented a dedicated Universal Feynman Output (`UFO`) model for quarkonia, named `sm_onia`, which employs a 4-flavour scheme (4FS), i.e. assuming the charm quark as massless and to be loaded for production of bottomonia. If charmonia are produced, it is necessary to type `sm_onia-c_mass` instead, to consider a 3FS with a massive charm quark. To generate a process with a J/ψ in the final state, for example, the user will type the following commands from the terminal in `MG5`:

```
MG5_aMC> import model sm_onia-c_mass
MG5_aMC> generate p p > Jpsi(1|3S11)
MG5_aMC> output; launch
```

This generates the process with the indicated Fock state in the command line. To generate the process for the physical bound state instead, the user can type

```
MG5_aMC> generate p p > Jpsi
```

which is equivalent to the commands

```
MG5_aMC> generate p p > Jpsi(1|3S11)
MG5_aMC> add process p p > Jpsi(1|1S08)
MG5_aMC> add process p p > Jpsi(1|3S18)
```

generating all three subprocesses together. The LDMEs are defined for each Fock state, and can be modified by the user directly in `onia_card.dat` right after launching. Having described shortly our implementation and discussed the user interface, we now show some results, first discussing the explicit benchmarks we have made against `Helac-Onia` [7, 8].

4. Results

We report some of the results obtained from the benchmarking against `Helac-Onia` and a set of various results that can be obtained with `MG5`. The benchmarking has been performed first checking the matrix-element squared, $|\mathcal{A}^{(N)}_{\{C,S\}}(r)|^2$, from both frameworks, evaluated at the same randomly-generated phase-space point. The exhaustive list of benchmarking we have performed is given in the supplementary file alongside the arXiv submission of our [2]. We have next benchmarked at the level of the cross section, σ, for a wide variety of processes, fixing identical input data, such as kinematic set-up and LDME values. We report as an example a few processes in table 1.

Our implementation handles processes with an arbitrary number of final-state quarkonia, in association with any elementary particles. We show in the following tables some selected results for various processes, including single, double and triple quarkonium final-state production. In each case, we also give the MC statistical uncertainty alongside our results.

These cross sections are meant to show the flexibility of the code: the hierarchy of the processes highly depends on the chosen LDMEs and the cuts applied are generic and do not correspond to any particular experimental set up. The user can set specific input data, depending on their needs. Indeed, the flexibility of the code allows the user to assign different LDMEs to Fock-state contributions on the fly, which is useful and intuitive, especially in cases where different Fock states can be studied.

Process	`MG5` `Helac-Onia`	**Process**	`MG5` `Helac-Onia`
$pp \to u\bar{u} \to J/\psi\left[{}^3S_1^{[8]}\right] + H$	42.055(2) yb	$pp \to gg \to J/\psi\left[{}^3S_1^{[8]}\right] + H$	1.8530(7) ab
	42.056(3) yb		1.8523(7) ab
$pp \to gg \to J/\psi\left[{}^3S_1^{[8]}\right] + HH$	15.927(3) yb	$pp \to gg \to J/\psi\left[{}^3S_1^{[8]}\right] + HHH$	1.9802(5) rb
	15.93(2) yb		1.967(4) rb

Table 1: A sample of cross-section results for processes with increasing H multiplicity. Results at the right of each process are obtained with both `MG5` (top result) and `Helac-Onia` (bottom one). Uncertainties from numerical MC integration on the last digit are shown in brackets.

Inclusive single charmonium and bottomonium production

As a first application of our new implementation, we compute the fully-inclusive LO cross section of four $2 \to 1$ processes involving a single quarkonium in pp collisions at 13 TeV, see Table 2.

process	σ	**process**	σ
$pp \to \eta_c + X$	2.9366(5) µb	$pp \to \eta_b + X$	5.4935(7) µb
$pp \to J/\psi + X$	536.14(6) nb	$pp \to \Upsilon + X$	6.0655(4) nb

Table 2: Total cross sections for single charmonium and bottomonium production in pp collisions at 13 TeV.

Associated charmonium and bottomonium production

Second, we consider a quarkonium produced alongside elementary particles, such as electroweak bosons, $W^\pm$ and Z, photons γ and also jets j. Some results are reported in Table 3 and are obtained using the following cuts: $p_{T,j} > 10$ GeV and $|\eta_j| < 5$ for the jet and $p_{T,\gamma} > 2$ GeV and $|\eta_\gamma| < 2.5$ for the photon.

process	σ	**process**	σ
$pp \to J/\psi + j + X$	329.8(2) nb	$pp \to \Upsilon + j + X$	19.85(1) nb
$pp \to \eta_c + \gamma + X$	789.3(4) pb	$pp \to \eta_b + \gamma + X$	2.257(1) pb

Table 3: A sample of fiducial cross sections for single charmonium and bottomonium production in pp collisions at 13 TeV, in association with a photon or jet (no feed-down effects nor experimental cuts).

Inclusive quarkonium-pair and triple-quarkonium production

Third, we consider a selection of processes with two final-state quarkonia. Our results are shown in Table 4. As a last example, we compute triple-J/ψ production to demonstrate the robustness of

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our implementation in handling larger multiplicity final states. We find,

$$\sigma(pp \to J/\psi + J/\psi + J/\psi + X) = 1.038(3)\ \text{pb}. \tag{10}$$

process	σ	**process**	σ
$pp \to \eta_c + \eta_c + X$	35.81(1) nb	$pp \to \eta_b + \eta_b + X$	75.64(3) pb
$pp \to \eta_c + J/\psi + X$	7.233(3) nb	$pp \to \eta_b + \Upsilon + X$	1.9244(6) pb
$pp \to J/\psi + J/\psi + X$	10.756(3) nb	$pp \to \Upsilon + \Upsilon + X$	44.63(1) pb

Table 4: Total cross sections for charmonium- and bottomonium-pair production in pp collisions at 13 TeV.

J/ψ production in association with a charm-anticharm pair

As a first application of our work with existing `MG5` features, we consider its interface with `Pythia8` [9] to parton shower (PS) events. We take the process $pp \to J/\psi + c\bar{c} + X$, generate events in the LHE format using our new implementation in `MG5` and interface them with `Pythia8` to perform the PS. For the analysis, we use the default settings of `Pythia8`, with initial-state radiation (ISR), final-state radiation (FSR), multiparton interactions (MPI) and hadronisation enabled, as well as taking the J/ψ to be a stable particle. Our results for the differential cross section as a function of the J/ψ transverse momentum $p_{T,J/\psi}$ at fixed-order and with the parton shower in place are shown in Figure 1.

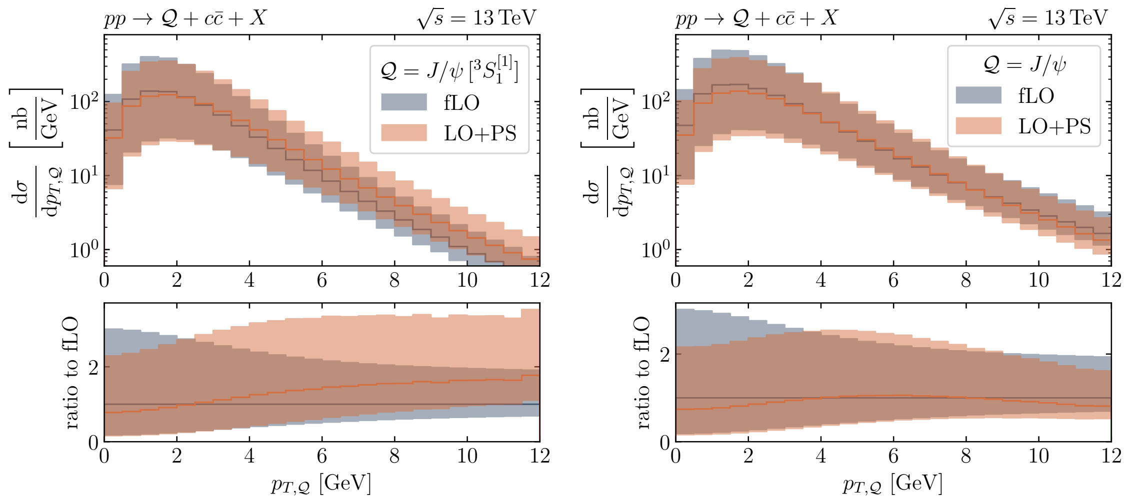

Figure 1: Differential cross section as a function of $p_{T,\mathcal{Q}}$ for the process $pp \to J/\psi + c\bar{c} + X$ at 13 TeV. We show results for production of the colour-singlet $J/\psi[^3S_1^{[1]}]$ Fock-state contribution (left panel) and the sum over all Fock-state contributions considered (right panel) with fixed LO (blue) and LO with PS (orange) contributions.

Quarkonium production in association with a Higgs boson

Another example of the flexibility of `MG5` is its capability to handle quarkonium-production processes

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not only within the SM. Our work maintains this feature and so we now consider the production of a vector quarkonium in association with a Higgs boson in pp collisions. To study this process with a $\Upsilon + H$ final state, we employ the HEFT within a new dedicated `UFO` model that can be imported with

```
MG5_aMC> import model heft_onia
MG5_aMC> generate g g > Upsilon H
```

For the J/ψ case, the user needs to replace the bottom-quark parameters with the charm-quark ones in `param_card.dat` and the corresponding LDME values in `onia_card.dat`.[1] The total cross-section results obtained for pp collisions, for both Υ and J/ψ, are

$$\begin{aligned} \sigma(pp \to gg \to J/\psi + H) &= 1.53^{+0.40}_{-0.29}\,\text{fb}\,, \\ \sigma(pp \to gg \to \Upsilon + H) &= 91^{+23}_{-17}\,\text{ab}\,. \end{aligned} \tag{11}$$

5. Conclusions and outlook

We have integrated quarkonium production in the `MadGraph5_aMC@NLO` framework, enabling automated cross-section computations for processes involving final-state S-wave bound states at LO in the NRQCD formalism. Our implementation supports a wide range of processes, i.e. production of single, multiple, and associated bound-state production in different kinematical environments in hadron-hadron, lepton-hadron and lepton-lepton collisions. We benchmarked our results against those of `Helac-Onia`, confirming the reliability of our implementation. We have produced cross-section results for a variety of processes, demonstrating the reach and potentiality of our extension, and illustrated the compatibility of our work with other `MG5` features, like its integration with `Pythia8` and user-defined Universal Feynman Output (`UFO`) models. We also remind that, even though in these proceedings the focus is put on quarkonium production only, this implementation encompasses leptonium and B_c production as well. Our work represents the first milestone of a broader project, including final-state P-wave bound states and, in the near future, an extension to NLO accuracy to facilitate state-of-the-art computations, allowing for a range of phenomenological applications including, for instance, global NRQCD analyses. Our implementation will be publicly available via the standard `MG5` distribution on launchpad (`https://launchpad.net/mg5amcnlo`) and on the NLOAcccess EU platform [10] (`https://nloaccess.in2p3.fr`).

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[1] There is no HEFT UFO model in the 3FS by default in `MG5`. Moreover, initial-state quark contributions are negligible for the process considered and so these modifications for J/ψ production is sufficient for our purposes.

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