Predictions for the isolated diphoton production through NNLO in QCD and comparison to the 8 TeV ATLAS data

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We present cross section predictions for the isolated diphoton production in next-to-next-to-leading order (NNLO) QCD using the computational framework MATRIX. Both the integrated and the differential fiducial cross sections are calculated. We found that the arbitrary setup of the isolation procedure introduces uncertainties comparable to the scale systematic errors. This fact is taken into account in the final result.

I. INTRODUCTION

Considerable attention, both experimental and theoretical, has been paid to the study of the diphoton productions. This process is relevant for testing the Standard Model predictions and is of great importance in Higgs studies. The diphoton final states is also important in new physics searches: the extra-dimensions, the supersymmetry and the new heavy resonances are three important topics among others.

The theoretical calculations are possible thanks to the codes DIPHOX [1], ResBos [2], 2γRes [3], 2γNNLO [4], MCFM [5] and recently MATRIX [6].

In addition to the direct production from the hard subprocess, photons can also come from the fragmentation subprocesses of QCD partons. The complete NLO one- and two-fragmentation contributions are implemented in DIPHOX. In ResBos only a simplified one-fragmentation contribution is considered but the resummation of initial-state gluon radiation to NNLL accuracy is included. Both DIPHOX and ResBos implement the gg →γγ component, to LO and NLO in QCD respectively. In the (NLO) MCFM calculations, the fragmentation component is implemented to LO accuracy.

Thanks to the high rate of production of final diphoton pairs (considered as relatively clean), experimentalists make precise measurements, pushing the experimental uncertainties down to the

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percent level, so that NLO calculations have become insufficient and therefore more precise investigations are required in order to reproduce the data and to provide a precise modeling of the SM backgrounds.

During the first run of the LHC (Run I), measurements of the production cross section for two isolated photons at a center-of-mass energy of $\sqrt{s} = 7$ TeV is performed by ATLAS [7] and CMS [8], based on an integrated luminosity of 4.9 fb$^{-1}$ and 5.0 fb$^{-1}$ respectively. This is concluded by ATLAS [9] at $\sqrt{s} = 8$ TeV using an integrated luminosity of 20.2 fb$^{-1}$ which gives a much more accurate result.

In Ref.[9], the authors reported that NLO calculations fail to reproduce the data and even if there is improvement of the result with $2\gamma$NNLO, it remains insufficient.

Although the NNLO isolated diphoton production cross sections can be calculated using the $2\gamma$NNLO and MCFM public codes, we used the most recent code MATRIX, because, in addition to its NNLO accuracy, it allows us to estimate systematic errors related to the $q_T$-subtraction procedure in an automatic way (see below).

Our work is organized as follows. In Sec-IIA, we give a short description of the MATRIX code. In Sec-IIB, we present the two isolation prescriptions used in the analysis. We describe a method which minimizes the difference between the results of both prescriptions and we propose a way to estimate this gap. In Sec-IIC, the NNLO cross section results are presented and compared to Data. We conclude in Sec-III.

II. NNLO CROSS SECTIONS

A. The Matrix code

The parton-level Monte Carlo generator MATRIX is a Fully differential computations in next-to-next-to-leading order (NNLO) QCD, it is based on a number of different computations and tools from various people and groups [6,10–15]. It achieves NNLO accuracy by using the $q_T$-subtraction formalism in combination with the Catani–Seymour dipole subtraction method. The systematic uncertainties inherent to the $q_T$-subtraction procedure can be controlled down to the few permille level or better for all NNLO predictions. To do this, a dimensionless cut-off $r_{cut}$ is introduced which renders all cross-section pieces separately finite and the power-suppressed contributions vanish in the limit $r_{cut} \to 0$. MATRIX simultaneously computes the cross section at several $r_{cut}$ values and then the extrapolated result is evaluated, including an estimate of the uncertainty of the extrapolation...
procedure, in an automatic way.

We can apply realistic fiducial cuts directly on the phase-space. The core of MATRIX framework is MUNICH Monte Carlo program [16], allowing us computing both QCD and EW corrections at NLO accuracy. The loop-induced $gg$ contribution entering at the NNLO is available for the diphoton production process.

### B. Isolation parameters

An isolation requirement is necessary to prevent contamination of the photons by hadrons produced during the collision, arising from the decays of $\pi^0, \eta, \text{etc.}$. Two prescriptions may be used for this purpose:

- the standard cone isolation criterion, used by collider experiments: a photon is assumed to be isolated if, the amount of deposited hadronic transverse energy $\sum_h E_T^h$ is smaller than some value $E_T^{\text{max}}$, inside the cone of radius $R$ in azimuthal $\phi$ and rapidity $y$ angle centered around the photon direction:

$$\sum_h E_T^h \leq E_T^{\text{max}}, \quad r = \sqrt{(\phi - \phi_\gamma)^2 + (y - y_\gamma)^2} \leq R.$$  

$E_T^{\text{max}}$ can be either a fixed value or a fraction $\varepsilon$ of the transverse momentum of the photon $p_T^\gamma$:

$$E_T^{\text{max}} = \text{const.} \quad \text{or} \quad E_T^{\text{max}} = \varepsilon p_T^\gamma, \quad 0 < \varepsilon \leq 1.$$  

$R$ and $E_T^{\text{max}}$ are chosen by the experiment; ATLAS and CMS use $R = 0.4$, but $E_T^{\text{max}}$ differs in their various measurements;

- the “smooth” cone or Frixione isolation criterion [17]: in this case $E_T^{\text{max}}$ is multiplied by a function $\chi(r)$ such that:

$$\begin{cases}
\lim_{r \to 0} \chi(r) = 0 \\
0 < \chi(r) < 1 \quad \text{if} \quad 0 < r < R
\end{cases}.$$  

a possible (and largely used) choice is

$$\chi(r) = \left[\frac{1 - \cos(r)}{1 - \cos(R)}\right]^n$$

so that:

$$\begin{cases}
\sum_h E_T^h \leq \chi \left[\frac{1 - \cos(r)}{1 - \cos(R)}\right]^n E_T^{\text{max}}, \\
r = \sqrt{(\phi - \phi_\gamma)^2 + (y - y_\gamma)^2} \leq R,
\end{cases}$$

(typically $n = 1$).
Despite the fact that the Frixione criterion (formally) eliminates all fragmentation contribution, it is not yet included in the experimental studies. On the other hand, the use of this criterion by the theoretical investigations of the diphoton production at NNLO is necessary to ensure the convergence of calculations and to produce efficient codes, since only the direct contribution is included.

In ATLAS measurement [9], the standard criterion is adopted for DIPHOX and ResBos but the “smooth” prescription is used for 2γNNLO, assuming $E_{T}^{\text{max}} = 11 \text{ GeV}$. This is far from the Les Houches accord 2013 recommendations which states that to match experimental conditions to theoretical calculations with reasonable accuracy, the isolation parameters must be tight enough: $E_{T}^{\text{max}} \leq 5 \text{ GeV}$ or $\varepsilon < 0.1$ (assuming $n = 1$) [18].

In Ref.[19], the authors present a rather complete study of the impact of the isolation parameters on the diphoton cross sections. Of this study, we can lift the following points:

- The NNLO cross sections are more sensitive to the variation of the parameters of isolation in comparison with the NLO results,
- at fixed $n = 1$, the total NNLO cross section for the “smooth” isolation increases by 6% in going from $E_{T}^{\text{max}} = 2$ to 10 GeV,
- considering the interval $0.5 < n < 2$, at fixed $E_{T}^{\text{max}} = 4 \text{ GeV}$, the total NNLO cross section with $n = 1$ increases by about 4% with $n = 0.5$ and decreases by about 5% with $n = 2$; the corresponding scale uncertainty is lesser than ±8.7%.

We notice that the isolation uncertainties due to the choice of the parameters of isolation are comparable to the scale uncertainties, thus we have to consider the arbitrary on the choice of these parameters as a major source of the theoretical systematic errors as well as uncertainties related to the choice of the scale. This must be included in the final result.

To evaluate these isolation uncertainties (i.e. to determine both the central value and deviations), we use MATRIX to calculate the NLO integrated cross sections by varying the parameters $n = 0, 0.1, 0.5, 1, 2, 4, 10$ and $E_{T}^{\text{max}} = 2, 3, 4, 5, 8, 11 \text{ GeV}$, then the results are compared to the NLO cross sections obtained by running the DIPHOX code using the standard isolation prescription with the same $E_{T}^{\text{max}}$ and $R$ parameters.

The so-called box (NNLO) contribution to the channel $gg \to \gamma\gamma$ is removed from the DIPHOX results to ensure that the comparison holds at the same NLO-order and the fine structure constant $\alpha$ is fixed to 1/137; the setup is summarised in Table [1] and results are shown in Fig. [12].
To minimise the difference between the isolation definitions used in the theoretical and the experimental analyses, the central value $\sigma_{\text{NLO}}$ is determined at the value $n = n_0$ such that:

$$\sigma_{\text{NLO}} \equiv \left(\sigma_{\text{NLO \, MATRIX}}^{n_0}\right) \simeq \sigma_{\text{DIPHOX}},$$

(6)

($R$ and $E_T^{\text{max}}$ fixed according to the isolation experimental requirement);

the isolation uncertainties are evaluated by varying $n$ from $\sim \frac{1}{2}n_0$ to $\sim 2n_0$. This procedure is adopted in the NNLO calculations (see Sec-IIC).

The “central value” of the parameter $n = n_0$ depends on the value of $E_T^{\text{max}}$ (see Table II), this is consistent with results of Ref. [19].

C. NNLO Results and comparison with data

We consider proton–proton collisions at the 8 TeV LHC. We choose the invariant mass of the photon pair as the central scale, i.e.

$$0 < \mu = m_{\gamma\gamma} < 1700 \, \text{GeV},$$

(7)

Frixione isolation with $0.5 < n < 2$, $E_T^{\text{max}} = 11 \, \text{GeV}$ and $R = 0.4$ (see Eq.(5)), and the following fiducial cuts:

$$p_T^{\gamma_1} > 40 \, \text{GeV}, \quad p_T^{\gamma_2} > 30 \, \text{GeV}, \quad |\eta^{\gamma_i}| < 2.37; \quad R_{\gamma\gamma} < 0.4;$$

(8)

excluding the gap region

$$1.37 < |\eta^{\gamma_i}| < 1.56.$$  

The fine structure constant $\alpha$ is fixed to $1/128.9$. Several modern NNLO PDF sets are used (CT14 [20], MMHT14 [21] and NNPDF3.1 [22]); the evolution of $\alpha_s$ at 3-loop order is provided by the corresponding PDF set.

for CT14, the central value of the NNLO integrated fiducial cross section is evaluated at the isolation parameters ($n = n_0 = 0.84$, $E_T^{\text{max}} = 11 \, \text{GeV}$) within the scale choice $\mu_R = \mu_F = m_{\gamma\gamma}$:

$$\left(\sigma_{\text{fid \, tot}}^{n=0.84}\right)^{\text{NNLO}} = 15.60 \pm 0.09 \, \text{(num)} \, \text{pb},$$

calculated at $r_{\text{cut}}$ extrapolated to zero.
The scale uncertainties are estimated in the usual way by independently varying $\mu_R$ and $\mu_F$ in the range
\begin{equation}
\frac{1}{2}m_{\gamma\gamma} \leq \mu_R, \mu_F \leq 2m_{\gamma\gamma},
\end{equation}
with the constraint
\begin{equation}
\frac{1}{2} \leq \frac{\mu_R}{\mu_F} \leq 2.
\end{equation}

The relative scale uncertainty in the integrated cross section is $(+6.7\%-5.6\%)$.

The relative isolation uncertainty is calculated by varying $n$ from 0.5 to 2:
\begin{align*}
\sigma_{n=0.5} - \sigma_{n=0.84} &\approx +3.8\% \\
\sigma_{n=2} - \sigma_{n=0.84} &\approx -5.5\%
\end{align*}

The impact of the variation of the strong coupling constant is also investigated. The change of $\alpha_s(M_Z^2)$ by $\pm 0.001$ from the central value 0.118 leads to variations $(+0.6\%-1.1\%)$ in the fiducial integrated cross section. The cross sections related to CT14, MMHT14 and NNPDF3.1 modern PDF sets are very close to each other with an uncertainty lesser than 0.4%.

We can write our theoretical prediction of the integrated fiducial cross section as:
\begin{align*}
\sigma_{\text{tot}}^{\text{fid}} &\approx 15.60 \pm 0.09 \text{ (num)} +6.7\% \text{ (scale)} +3.8\% \text{ (iso)} \\
&\approx 15.60 \pm 0.09 \text{ (num)} +1.05\% \text{ (scale)} +0.59\% \text{ (iso)} \\
&\approx 15.60_{-1.24}^{+1.21} \approx (15.6 \pm 1.2) \text{ pb}
\end{align*}

which is consistent with the experimental data $(16.8 \pm 0.8) \text{ pb}$.

Note that the theoretical uncertainties are dominated by both scale and isolation systematic errors which are of the same order.

Since this process involves isolated photons in the final state it has a relatively large numerical uncertainty at NNLO after the $r_{\text{cut}} \to 0$ extrapolation, and as recommended by authors of Ref.[6], the distribution calculated at fixed $r_{\text{cut}} = 0.05\%$ must be multiplied by the correction factor:
\begin{equation}
\frac{(\sigma_{\text{tot}}^{\text{fid}})_{r_{\text{cut}} \to 0}}{(\sigma_{\text{tot}}^{\text{fid}})_{r_{\text{cut}} = 0.05\%}} \approx 0.98.
\end{equation}

The MATRIX differential cross section is consistent with data as shown in Fig. 3-4.
III. CONCLUSION

We present the calculation of the integrated and differential cross sections for the isolated diphoton production in pp collisions at the centre–of–mass energy $\sqrt{s} = 8$ TeV in next-to-next-to-leading order (NNLO) QCD using the computational framework MATRIX. A special care is paid to the choice of the Frixione isolation parameters. We keep the same value of $E_T^{\text{max}} = 11$ GeV and $R = 0.4$ used by experimentalists but we adjust the value of the parameter $n$ until the integrated cross section calculated by MATRIX matches that calculated by DIPHOX at the same NLO-order (without the $Box$-contribution to the channel $gg \rightarrow \gamma\gamma$).

Once these parameters fixed, we calculate the central value of the MATRIX (NNLO) cross sections and by varying the Frixione parameter $n$ from 0.5 to 2, we estimate the relative isolation uncertainty $\left(\frac{+3.8\%}{-5.5\%}\right)$. The scale uncertainty is found to be equal to $\left(\frac{+6.7\%}{-5.7\%}\right)$.

Both the scale and the isolation uncertainties are of the same order and represent the main source of the theoretical errors, the uncertainties inherent to the $q_T$-subtraction procedure ($\sim 0.6\%$) and to the variation of the coupling constant $\alpha_s(M_Z^2)$ ($\sim 0.8\%$) are negligible.

Our predictions for the differential and the integrated cross sections are in good agreement with the data, in particular we have $\sigma_{\text{tot}}^{\text{fid}} \simeq 15.60 \pm 0.09 \, (\text{num}) \, +6.7\% \, (\text{scale}) \, +3.8\% \, (\text{iso}) \simeq (15.6 \pm 1.2) \, \text{pb}$.

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Table I: Setup of the diphoton production process used in the NLO runs.

| $p_T^\gamma$ (GeV) | $m_{\gamma\gamma}$ (GeV) | $E_{T}^{\text{max}}$ (GeV) | $\eta_\gamma$ | $\sigma_{\text{NLO}}^\text{MATRIX}$ (pb) |
|---------------------|---------------------|-----------------|----------|-----------------|
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 11$ GeV | $0.84$ | $13.78 \pm 0.12$ (num) $^{+6.1\%}_{-5.0\%}$ (scale) |
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 8$ GeV | $1.2$ | $13.36 \pm 0.10$ (num) $^{+5.9\%}_{-4.8\%}$ (scale) |
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 5$ GeV | $2.0$ | $13.01 \pm 0.10$ (num) $^{+5.8\%}_{-4.7\%}$ (scale) |
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 4$ GeV | $3.2$ | $13.69 \pm 0.11$ (num) $^{+5.7\%}_{-4.6\%}$ (scale) |
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 3$ GeV | - | - |
| $25 > p_T^\gamma,$ $|\eta_\gamma| < 2.37;$ | $80 < m_{\gamma\gamma} < 1700$ GeV | $E_{T}^{\text{max}} < 2$ GeV | - | - |

Table II: The “central value” of the parameter $n = n_0$. 

Figure 1: The MATRIX integrated fiducial cross section $\sigma_{\text{NLO}}^\text{MATRIX}$ as a function of the parameter $n$ related to Frixione isolation criterion (see Eq. 5) for different values of $E_{T}^{\text{max}}$. 
Figure 2: The MATRIX and the DIPHOX integrated fiducial cross section $\sigma_{NLO}^{\text{tot}}$ as a function of the parameter $n$ related to Frixione isolation criterion (see Eq.5) for several values of $E_T^{\text{max}}$. The “central value” of the parameter $n = n_0$ depends on the value of $E_T^{\text{max}}$, they are reported in Table II.
Figure 3: The MATRIX differential fiducial cross section related to CT14 as a function of $m_{\gamma\gamma}$ compared to the data [9].
Figure 4: The MATRIX differential fiducial cross section related to CT14 as a function of $m_{\gamma\gamma}$ compared to the data [9], in the range $0 < m_{\gamma\gamma} < 250 \text{ GeV}$. 