Chapter 4

Diphoton Production

4.1 Introduction

Improved theoretical predictions to higher orders in QCD have been performed for cross sections of pair production processes *viz.* di-lepton [50, 51, 52], di-gauge boson (γγ [56, 57], ZZ [59] and W+W− [60]), which in the LED model could result from the exchange of a virtual KK mode in addition to the usual SM contribution. The real emission of KK modes lead to large missing $E_T$ signals *viz.*, mono-jet [92], mono-photon [93], mono-Z boson and mono-$W^\pm$ boson [106, 107]. NLO QCD corrections in some of the above processes are quite substantial and their inclusion in the computation also lead to a reduction of theoretical uncertainties, making it possible for the experiments to put more stringent bounds on the extra dimension model parameters.

The diphoton final state is an important signal for extra dimension searches, as the branching ratio of a KK mode decay to diphoton is twice than that of a decay to individual charged lepton pair. The quantitative impacts of the NLO QCD correction to the diphoton final state for extra dimension searches have been studied
in [56, 57], where various IR safe observables were studied using phase space slicing method. The factorisation scale dependence gets reduced when $\mathcal{O}(\alpha_s)$ corrections are included. Fixed order calculation truncated to NLO, at best yields results for sufficiently inclusive observable. Combining fixed order NLO and PS Monte Carlo [32, 33], would extend the coverage of the kinematical region to consistently include resummation in the collinear limit and also produce a more exclusive description of the final state to make it as realistic as possible to the experimental situation. The flexibility to incorporate hadronisation models and capabilities to simulate realistic final state configurations, that can undergo detector simulations, are the main advantages for the experimental collaborations.

ATLAS [76] and CMS [75] have analysed the diphoton invariant mass spectrum, using a constant K-factor for the full range of the invariant mass distribution to put lower bounds on extra dimension scale to NLO accuracy. However, this choice is not sensitive to possible distortions of distributions that can arise at NLO. Our present analysis will further help to put more stringent bounds on the model parameters. Bounds on $M_S$ for different extra dimensions d have been obtained by ATLAS and CMS collaborations [75, 76]. For our present analysis, we choose the following values: $M_S = 3.7 \text{ TeV (d=2)}, 3.8 \text{ TeV (d=3)}, 3.2 \text{ TeV (d=4)}, 2.9 \text{ TeV (d=5)}, 2.7 \text{ TeV (d=6)}$. For relevant observables, we consider the fixed order results to NLO accuracy and include PS. Factorisation, renormalisation scale uncertainties and PDF uncertainties are also estimated in an automated way [108]. For photon isolation, both smooth cone isolation and the experimental isolation criteria are considered.
4.2 NLO+PS

Since the KK modes couple universally to the SM particles through the energy momentum tensor, both the $q\bar{q}$ and $gg$ channel would contribute to the diphoton final state at leading order (LO). In the SM, the $gg$ channel starts only at NNLO level via the finite box contribution through quark loop and the large gluon-gluon flux at the LHC makes this contribution potentially comparable to the LO results. In the invariant mass region of interest to extra dimension searches, the box diagram contribution is not significant enough [56, 57].

All the partonic contributions to NLO in QCD have been calculated for the diphoton final state [56, 57], for both ADD [36, 37, 38] and RS [42] extra dimension models. QCD radiative corrections through virtual one loop gluon and real emission of gluons to the $q\bar{q} \rightarrow \gamma \gamma$ subprocess, would contribute to both SM and extra dimension models. The $q(\bar{q}) g \rightarrow q(\bar{q}) \gamma \gamma$ begins to contribute for both SM and extra dimension models at NLO. The LO $g g \rightarrow \gamma \gamma$ extra dimension process will also get one loop virtual gluon and real gluon emission radiative corrections. There will also be interference between the SM and extra dimension model to give contributions up to $O(\alpha_s)$ and in this analysis all of them are taken care of. We have included the $O(\alpha_s)$ corrections as a result of the interference between the SM box diagram contribution and LO extra dimension contribution to the $g g \rightarrow \gamma \gamma$ subprocess for completeness, though it is quite suppressed in the region of interest to extra dimension models and contributes only about 0.1% to the $gg$ subprocess.

The $q(\bar{q}) g \rightarrow q(\bar{q}) \gamma \gamma$ NLO contribution has an additional QED collinear singularity when the photon gets collinear to the emitting quark and can be absorbed into the fragmentation function which gives the probability of a parton fragmenting into a photon. Parton fragmentation functions are additional non perturbative inputs which are not very well known. At the LHC, secondary photons as a result of hadron
decaying into collinear photons and jets faking as photon are taken care of by photon isolation criteria [75, 76] which also substantially reduces the fragmentation contribution. Since the fragmentation is essentially a collinear effect, the fragmentation function can be avoided by the smooth cone isolation proposed by Frixione [109], which ensures that in no region of the phase space the soft radiation is eliminated. The smooth cone isolation is able to eliminate the not so well known fragmentation contribution and at the same time, it ensures IR safe observable. Centered in the direction of the photon in the pseudo rapidity (η) and azimuthal angle (φ) plane, a cone of radius \( r = \sqrt{(\eta - \eta_{\gamma})^2 + (\phi - \phi_{\gamma})^2} \) is defined. The hadronic activity \( H(r) \) is defined as the sum of hadronic transverse energy in a circle of radius \( r < r_0 \) and \( E_{T\gamma} \) is the transverse energy of the photon. For all cones with \( r \leq r_0 \), the isolation criterion \( H(r) < H(r)_{\text{max}} \) has to be satisfied, where \( H(r)_{\text{max}} \) is defined as,

\[
H(r)_{\text{max}} = \epsilon_{\gamma} E_{T\gamma} \left( \frac{1 - \cos r}{1 - \cos r_0} \right)^n. \tag{4.1}
\]

Efforts for the experimental implementation of the smooth cone isolation is on going.

Automation is an essential ingredient of this work. We have chosen to work in the AMCATNLO framework [110], which automatises the MC@NLO formalism [32] to match NLO computations with parton showers. In this chapter, we present results matched to HERWIG [16]. For the NLO computation, isolation of IR poles and phase space integration are carried out by MadFKS [111], which automatises the FKS subtraction method [112] using the MadGraph [113] matrix-element generator, whereas for one-loop amplitudes the results of [56, 57] are used. The automation within the MadGraph framework requires a new HELAS [114] subroutine to calculate helicity amplitudes with massive spin-2 particles [115, 116]. In addition, for our present analysis, we have implemented the sum over the KK modes of the virtual
graviton (see eq. (1.10)) in it (see Appendix D for details). We use this framework to
generate the events for 8 TeV run at the LHC. For the invariant mass distributions
we have reproduced the results of [56, 57] using the fixed order results obtained from
this set-up. Also numerical cancellation of the singularities from the real and virtual
terms have been explicitly checked.

Figure 4.1: Transverse momentum ($P_{T\gamma\gamma}$) distributions of the diphoton for the fixed
order NLO and NLO+PS. The ADD model parameters used are $d = 2$ and $M_S = 3.7$
TeV. The lower inset displays the fractional scale and PDF uncertainties of the
NLO+PS (ADD) results.

4.3 Numerical Results

In this section, we present the results for various kinematic distributions of photon
pair in SM and ADD model. We have included all the subprocess contributions to
NLO. The following input parameters are used: $\alpha_{em}^{-1} = 132.507$, $G_F = 1.16639 \times 10^{-5}$
Figure 4.2: Invariant mass ($M_{\gamma\gamma}$) distributions for ATLAS (left panel) and CMS (right panel) for $d = 2$ and $M_S = 3.7$ TeV. The SM contribution to NLO+PS and ADD to LO+PS and NLO+PS have been plotted. For the NLO+PS (ADD) results, the lower insets display the fractional scale and PDF uncertainties.

Our calculation is LO in the electroweak coupling and therefore the dependence on the scale in this coupling constant is beyond the precision of our results. In our electroweak scheme, $m_W$ and $\sin^2 \theta_W$ are computed from $m_Z$, $\alpha_{em}$ and $G_F$; this value for the $\alpha_{em}$ gives a W-boson mass ($m_W = 80.419$ GeV) that is close to the experimental value. The MSTW PDF also sets the value of the strong coupling $\alpha_s(m_Z)$ at LO and NLO in QCD. The renormalisation and factorisation scales are chosen as $\mu_F = \mu_R = M_{\gamma\gamma}$, the invariant mass of the photon pair. The events that have to be showered are generated using the following generation cuts: $|\eta_{1,2}| < 2.6$, $P_T^{\gamma_1,\gamma_2} > 20$ GeV, diphoton invariant mass $100$ GeV < $M_{\gamma\gamma}$ < $M_S$ and the photon
isolation is done using the Frixione isolation with \( r_0 = 0.38, \epsilon_\gamma = 1 \) and \( n = 2 \). More specific analysis cuts are applied subsequently while showering the events in order to produce unbiased results.

The dependence of the prediction of an observable on the factorisation and renormalisation scales, is a result of the uncalculated higher order contributions, which can be estimated by varying \( \mu_F \) and \( \mu_R \) independently around the central value \( \mu_F = \mu_R = M_{\gamma\gamma} \). The variation is done by the following assignment \( \mu_F = \xi_F M_{\gamma\gamma} \) and \( \mu_R = \xi_R M_{\gamma\gamma} \), where the values for \((\xi_F, \xi_R)\) used are \((1,1)\), \((1/2,1/2)\), \((1/2,1)\), \((1,1/2)\), \((1,2)\), \((2,1)\), \((2,2)\). The various ratios of \( \mu_F, \mu_R \) and \( M_{\gamma\gamma} \) that appear as arguments of logarithms in the perturbative expansion to NLO are within the range \([1/2,2]\]. The variation of both \( \mu_F \) and \( \mu_R \) are taken as the envelope of the above individual variations. Variation of only \( \mu_F \) would involve the choice \( \xi_R = 1 \) & varying \( \xi_F \) and vice-versa for variation of only \( \mu_R \). The PDF uncertainties are estimated in the Hessian method using the prescription given by MSTW [117]. Fractional uncertainty defined as the ratio of the variation about the central value divided by the central value, is a good indicator of the scale and PDF uncertainties and is plotted in the lower insets of various figures. As described in [108], the generation of these uncertainty bands can be done at virtually no extra CPU cost within the AMC@NLO framework.

To begin with, we compare the fixed order NLO result with NLO+PS for the transverse momentum of the diphoton \( \log_{10} P^\gamma_T \) using ‘generic’ cuts: \( M_{\gamma\gamma} > 140 \) GeV, \(|\eta_\gamma| < 2.5\), \( P_T^{\gamma_1} > 40 \) GeV, \( P_T^{\gamma_2} > 25 \) GeV and \( r_0 = 0.4 \). In Fig. 4.1, \( \log_{10} P_T^{\gamma\gamma} \) distribution is plotted for \( d = 2 \) with appropriate \( M_S \) value. It is clear that at low \( P_T^{\gamma\gamma} \) values, NLO+PS correctly resums the Sudakov logarithms, leading to a suppression of the cross section, while the fixed order NLO result diverges for \( P_T^{\gamma\gamma} \to 0 \). At high \( P_T^{\gamma\gamma} \), the NLO fixed order and NLO+PS results are in agreement. In the lower inset
of Fig. 4.1, we have presented the scale and PDF variations of the NLO+PS, which increase with $P_T^{\gamma\gamma}$ as observed in [118].

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig43}
\caption{Invariant mass ($M_{\gamma\gamma}$) distributions for $d = 3$ (left panel) and $d = 4$ (right panel) are plotted for ADD and SM contributions to NLO+PS accuracy. The lower insets give the corresponding fractional scale and PDF uncertainties for NLO+PS (ADD).}
\end{figure}

We now present the results for the various kinematical distributions to NLO accuracy with PS (labelled as NLO+PS), for analysis specific cuts. Both the experiments ATLAS and CMS have looked for diphoton invariant mass in the region $140 \text{ GeV} < M_{\gamma\gamma} < M_S$. ATLAS cuts [76]: the rapidity of the individual photons are in the region $|\eta_{\gamma}| < 2.37$, with an exclusion region $1.37 < |\eta_{\gamma}| < 1.52$, the transverse momentum of the individual photons $P_{T\gamma} > 25 \text{ GeV}$ and for photon isolation: sum of transverse energy of hadrons $\sum E_T(H) < 5 \text{ GeV}$ with $\Delta r < 0.4$, where $\Delta r = \sqrt{\Delta \phi^2 + \Delta \eta^2}$ is a cone in the rapidity – azimuthal angle plane. For CMS the
corresponding cuts are [75]: $|\eta_\gamma| < 1.44$, $P_T^\gamma > 70$ GeV, photon isolation: (i) sum of the energy of hadrons $\sum E(H) < 0.05 E^\gamma$ with $\Delta r < 0.15$, (ii) sum of transverse energy of hadrons $\sum E_T^H < 2.2$ GeV + $0.0025 E_T^\gamma$ with $0.15 < \Delta r < 0.4$. We have further checked that, in addition to the ATLAS and CMS photon isolation, if we also include the Frixione isolation criteria, there are no appreciable changes in the final results.

In Fig. 4.2, we have plotted invariant mass distributions $d\sigma/dM_{\gamma\gamma}$ of photon pair in the SM as well as in the ADD model for ATLAS (left panel) and CMS (right panel). For ADD model we have obtained the distributions for $M_S = 3.7$ TeV and $d = 2$. The central value curves correspond to the choice $\mu_F = \mu_R = M_{\gamma\gamma}$, have been plotted for the ADD (NLO+PS) and purely SM (NLO+PS) contribution. The label ADD refers to the total contribution coming from SM, ADD and the interference between them. The corresponding ADD (LO+PS) contribution gives an indication of the quantitative impact of the NLO QCD correction. At larger invariant mass of the photon pair, the ADD effect is dominant. To demonstrate the sensitivity of our predictions to the choice of scale and PDF uncertainties, in the lower insets fractional uncertainties by varying (a) both $\mu_F$ and $\mu_R$ and (b) PDF error sets, are plotted. The difference in the distributions in Fig. 4.2 for ATLAS and CMS can be attributed to the very different cuts used for their analysis. In Fig. 4.3, the corresponding plots for $d = 3, 4$ are plotted for the CMS cuts. The choice of $M_S$ used for the plots corresponds to the lower bounds obtained by [75, 76] using the diphoton process. By including higher order corrections, the scale dependence goes down from about 25% at LO, to about 10% at NLO, as can be estimated from the ratio plots. The PDF uncertainty does not change significantly and remains about 8%.

We now consider the fractional scale uncertainties on the invariant mass dis-
Figure 4.4: For the invariant mass distribution with $d = 2$ and $M_S = 3.7$ TeV, the fractional scale uncertainties as a result of $\mu_F$ variation (upper left panel), $\mu_R$ variation (upper right panel) and $\mu_F$, $\mu_R$ variation (lower panel).

...
mass factorisation. As expected the inclusion of NLO QCD correction reduces the factorisation scale dependence resulting from the LO observable which is clear from Fig. 4.4 (upper left panel). In the high $M_{\gamma\gamma}$ region, the uncertainty of about 25% at LO+PS gets reduced to 5% when NLO+PS corrections are included. On the other hand, the $\mu_R$ dependence enters only at NLO level (see upper right panel of Fig. 4.4) which will get reduced only if NNLO corrections are included. Hence, we see our NLO corrections are sensitive to the choice of $\mu_R$ but the variation is only 5% and is fairly constant for the range of invariant mass considered. If we vary both $\mu_F$ and $\mu_R$ simultaneously as shown in Fig. 4.4 (lower panel), we find that the reduction in the $\mu_F$ scale dependence at NLO level is mildly affected by the $\mu_R$ variation in the
large invariant mass region. In the small invariant mass region, the LO and NLO results exhibit smaller $\mu_F$ dependence compared to the large invariant mass region. But $\mu_R$ dependence coming from the NLO results does not change much with the invariant mass $M_{\gamma\gamma}$. Hence variation due to $\mu_R$ at small $M_{\gamma\gamma}$ is larger compared to that resulting from $\mu_F$. This explains the behavior at small invariant mass regions where the NLO+PS variation is in excess of the LO+PS (see lower panel of Fig. 4.4).

Figure 4.6: Transverse momentum ($P_T^{\gamma\gamma}$) distributions of the diphoton for $d = 3$ (left panel) and $d = 4$ (right panel) along with the corresponding fractional scale and PDF uncertainties (lower inset) of the NLO+PS (ADD) results.

The rapidity ($Y$) distribution of the diphoton pair is plotted in Fig. 4.5 for $d = 3$ (left panel) and $d = 4$ (right panel). For this analysis we have chosen $M_{\gamma\gamma} > 600$ GeV, the region where the effects of ADD model begins to dominate over the SM diphoton signal at NLO (see Fig. 4.3). The scale and PDF uncertainties to NLO are displayed as insets at the bottom of each figure. The scale uncertainties are
usually larger than the PDF uncertainties in the rapidity distribution except for the
central rapidity region where they are comparable. For $d = 3$ the scale uncertainties
are about 20% around the central rapidity region, which come down to about 10%
when NLO+PS corrections are included. The PDF uncertainties for LO+PS and
NLO+PS are comparable.

Finally, we plot the transverse momentum distribution in Fig. 4.6 for $d = 3$ (left
panel) and $d = 4$ (right panel), for the SM and ADD model to NLO+PS accuracy,
with $M_{\gamma\gamma} > 600$ GeV. The ADD results are also plotted for LO+PS. The scale and
PDF uncertainties are displayed as insets at the bottom of the plots for NLO+PS
(ADD).

4.4 Conclusion

In this chapter, we have presented the diphoton final state in the LED model to
NLO in QCD and matching to PS is implemented using the AMC@NLO frame-
work. All the subprocesses that contribute to the diphoton final state from both the
SM and ADD model are considered to NLO in QCD. This is the first time MC@NLO
formalism has been used for a processes in the ADD model and we hope it would
significantly help extra dimension searches at the LHC to constrain the ADD model
parameters. Using a set of generic cuts, we first demonstrated the importance of
NLO+PS over the fixed order NLO computations, by considering the $P_T^{\gamma\gamma}$ dis-
bution. We have presented our results for various observables viz., invariant mass,
rapidity and transverse momentum of the diphoton, both for the ATLAS and CMS
detector specific cuts to NLO+PS accuracy. It is important to note that there is
substantial enhancement of the various distributions due to the inclusion of NLO
corrections and both the theoretical and PDF uncertainties have been estimated.
There is a significant decrease in theoretical uncertainties from over 20% at LO to about 10% when NLO corrections are included. The results are presented for different number of extra spatial dimensions $d = 2 - 6$ with respective values of the fundamental scale $M_S$ that have been experimentally bounded. The event files for $d = 2-6$ are available on the website http://amcatnlo.cern.ch. Nevertheless, the complete code is also uploaded on the website http://amcatnlo.cern.ch so that it could be used by the experimental collaborations in the large extra dimension searches at the LHC.