$gg \rightarrow HH$: Combined uncertainties

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In this paper we discuss the combination of the usual renormalization and factorization scale uncertainties of Higgs-pair production via gluon fusion with the novel uncertainties originating from the scheme and scale choice of the virtual top mass. Moreover, we address the uncertainties related to the top-mass definition for different values of the trilinear Higgs coupling and their combination with the other uncertainties.

I. INTRODUCTION

Higgs-boson pair production will allow for the first time to probe the trilinear Higgs self-coupling directly and, thus, to determine the first part of the Higgs potential as the origin of electroweak symmetry breaking. The dominant Higgs pair production mode is a gluon fusion $gg \rightarrow HH$ that is loop induced at leading order (LO), mediated by the top and, to a much lesser extent, bottom loops [1]. The total gluon-fusion cross section is about 3 orders of magnitude smaller than the corresponding single-Higgs production cross section [2]. The dependence of the gluon-fusion cross section on the trilinear Higgs self-coupling λ around the Standard Model (SM) value is approximately given by $\Delta\sigma/\sigma \sim -\Delta\lambda/\lambda$ so that the uncertainties of the cross section are immediately translated into the uncertainty of the extracted trilinear self-coupling. In order to reduce the uncertainties of the cross section higher-order corrections are required. The next-to-leading-order (NLO) QCD corrections have first been obtained in the heavy-top limit (HTL) [3] supplemented by a large top-mass expansion [4] and the inclusion of the full real corrections [5]. Meanwhile, the full NLO calculation including the full top-mass dependence has become available [6–8] showing a 15% difference to the result obtained in the HTL for the total cross section. For the distributions, the differences can reach 20–30% for large invariant Higgs pair masses. The full NLO results have been confirmed by suitable

expansion methods [9]. Within the HTL the next-to-NLO (NNLO) [10] and next-to-NNLO (N³LO) [11], QCD corrections have been derived and raise the cross section by a moderate amount of 20–30% in total. The complete QCD corrections increase the cross section by more than a factor of 2. Quite recently, the full NLO result and the NNLO corrections in the HTL have been combined in a fully exclusive Monte Carlo program [12] (including the mass effects of the one-loop double-real contributions at NNLO) that is publicly available.[1] Moreover, the matching of the full NLO results to parton showers has been performed [13] so that there are complete NLO event generators.

II. UNCERTAINTIES

The usual renormalization and factorization scale uncertainties at NLO amount to about 10–15% [6,8],

$$\sqrt{s} = 13 \text{ TeV}: \sigma_{\text{tot}} = 27.73(7)^{+13.8\%}_{-12.8\%} \text{ fb},$$
$$\sqrt{s} = 14 \text{ TeV}: \sigma_{\text{tot}} = 32.81(7)^{+13.5\%}_{-12.5\%} \text{ fb},$$
$$\sqrt{s} = 27 \text{ TeV}: \sigma_{\text{tot}} = 127.0(2)^{+11.7\%}_{-10.7\%} \text{ fb},$$
$$\sqrt{s} = 100 \text{ TeV}: \sigma_{\text{tot}} = 1140(2)^{+10.7\%}_{-10.0\%} \text{ fb}, \quad (1)$$

where s denotes the squared center-of-mass energy and σ_{tot} the total cross section. The numbers in brackets are the numerical integration errors and the upper and lower percentage entries denote the combined renormalization and factorization scale uncertainties. They have been obtained by a (7-point) variation of the renormalization and factorization scales μ_R, μ_F by a factor of 2 around the central (dynamical) scale $\mu_0 = M_{HH}/2$, where M_{HH}

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[1]The approach of Ref. [12] is called NNLO$_{\text{FTapprox}}$.

denotes the invariant Higgs-pair mass. The numbers of Eq. (1) have been obtained for a top pole mass of $m_t = 172.5$ GeV, a Higgs mass of $M_H = 125$ GeV, and PDF4LHC parton distribution functions (PDFs) [14]. However, in addition to the scale dependence of the strong coupling constant and the PDFs, the virtual top mass is subject to a scheme and scale dependence, too. This involves the top mass included in the top Yukawa coupling, as well as the top mass entering the virtual top propagators.

The (central) numbers of Eq. (1) are obtained in terms of the top pole mass. In order to derive the corresponding results with the top $\overline{\text{MS}}$ mass $\bar{m}_t$ for both the Yukawa coupling and propagator mass, we use the N³LO relation between the pole and $\overline{\text{MS}}$ mass

$$\bar{m}_t(m_t) = \frac{m_t}{1 + \frac{4}{3}\frac{\alpha_s(m_t)}{\pi} + K_2\left(\frac{\alpha_s(m_t)}{\pi}\right)^2 + K_3\left(\frac{\alpha_s(m_t)}{\pi}\right)^3} \quad (2)$$

with $K_2 \approx 10.9$ and $K_3 \approx 107.11$. The scale dependence of the $\overline{\text{MS}}$ mass is treated at next-to-next-to-next-to-leading logarithmic level (N³LL),

$$\bar{m}_t(\mu_t) = \bar{m}_t(m_t)\frac{c[\alpha_s(\mu_t)/\pi]}{c[\alpha_s(m_t)/\pi]} \quad (3)$$

with the coefficient function [15]

$$c(x) = \left(\frac{7}{2}x\right)^{\frac{4}{7}}[1 + 1.398x + 1.793x^2 - 0.6834x^3]. \quad (4)$$

This introduces a new scale μ_t, the dependence on which induces an additional uncertainty. For large values of the invariant Higgs-pair mass, the high-energy expansion of the virtual form factors clearly favors the dynamical scale choice $\mu_t \sim M_{HH}$ [8,16].

The scale dependence of the total and differential Higgs-pair production cross section on μ_t drops by roughly a factor of 2 from LO to NLO as explicitly described in Ref. [8]. The procedure to obtain the associated uncertainties is to take the envelope of the different predictions with the top pole mass and the $\overline{\text{MS}}$ mass $\bar{m}_t(\mu_t)$ at the scale $\mu_t = \bar{m}_t$ and varying it between $M_{HH}/4$ and M_{HH} (i.e., a factor of 2 around the central renormalization and factorization scale $\mu_R = \mu_F = M_{HH}/2$ for each M_{HH} bin and integrating the maxima/minima eventually. At NLO we are left with the residual uncertainties related to the top-mass scheme and scale choice [7,8],

$$\sqrt{s} = 13 \text{ TeV}: \sigma_{\text{tot}} = 27.73(7)^{+4\%}_{-18\%} \text{ fb,}$$
$$\sqrt{s} = 14 \text{ TeV}: \sigma_{\text{tot}} = 32.81(7)^{+4\%}_{-18\%} \text{ fb,}$$
$$\sqrt{s} = 27 \text{ TeV}: \sigma_{\text{tot}} = 127.8(2)^{+4\%}_{-18\%} \text{ fb,}$$
$$\sqrt{s} = 100 \text{ TeV}: \sigma_{\text{tot}} = 1140(2)^{+3\%}_{-18\%} \text{ fb.} \quad (5)$$

A further reduction of these uncertainties can only be achieved by the determination of the full mass effects at

NNLO, which is beyond the state of the art.[2] Since these uncertainties are sizeable, the question arises of how to combine them with the other renormalization and factorization scale uncertainties of Eq. (1).

The interplay of the different uncertainties of Eqs. (1) and (5) at NLO is very simple, i.e., defining the envelope of all uncertainties leads to a *linear* addition of the renormalization and factorization scale uncertainties of Eq. (1) and the top-mass scheme and scale uncertainties of Eq. (5) since the latter turn out to be (nearly) independent of the renormalization and factorization scale choices. This statement has been evaluated up to NLO explicitly.

The presently recommended predictions and uncertainties are based on the work of Ref. [12]. This work includes the NNLO QCD corrections in the HTL combined with the full mass effects of the LO and NLO predictions. Moreover, the work includes the full mass dependence of the one-loop double-real corrections at NNLO. The central values and residual renormalization and factorization scale uncertainties of this approach are given by [12,17]

$$\sqrt{s} = 13 \text{ TeV}: \sigma_{\text{tot}} = 31.05^{+2.2\%}_{-5.0\%} \text{ fb,}$$
$$\sqrt{s} = 14 \text{ TeV}: \sigma_{\text{tot}} = 36.69^{+2.1\%}_{-4.9\%} \text{ fb,}$$
$$\sqrt{s} = 27 \text{ TeV}: \sigma_{\text{tot}} = 139.9^{+1.3\%}_{-3.9\%} \text{ fb,}$$
$$\sqrt{s} = 100 \text{ TeV}: \sigma_{\text{tot}} = 1224^{+0.9\%}_{-3.2\%} \text{ fb.} \quad (6)$$

These uncertainties will be further reduced by consistently including the novel N³LO corrections in the HTL [11].

III. COMBINATION OF UNCERTAINTIES

In order to find a proper scheme to combine the renormalization and factorization scale uncertainties of Eq. (6) and the uncertainties originating from the top-mass scheme and scale choice of Eq. (5), we have to consider the systematics of these uncertainties in more detail. Each perturbative order of the total (and differential) cross section in QCD can be decomposed in two different pieces of the corrections,

$$d\sigma_n = \sum_{i=0}^{n} d\sigma^{(i)}$$
$$d\sigma_n = d\sigma_{n-1} \times (K_{\text{SVC}}^{(n)} + K_{\text{rem}}^{(n)}), \quad (7)$$

where $d\sigma_n$ denotes the nth-order-corrected differential cross section, $d\sigma^{(i)}$ the ith-order correction, $K_{\text{SVC}}^{(n)}$ the universal part of the soft + virtual + collinear corrections, and $K_{\text{rem}}^{(n)}$ the remainder of the nth-order corrections relative to the previous order of the cross section. The (top-mass

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[2]Due to the moderate size of the NNLO corrections, a reduction of these uncertainties by a factor ~3–4 may be expected by the NNLO mass effects.
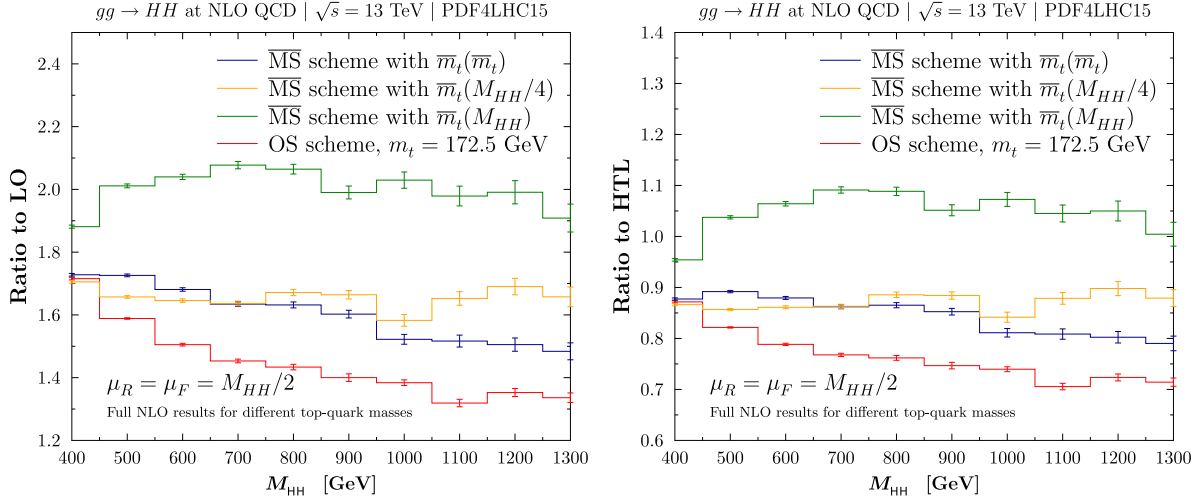
FIG. 1. Ratio of the full NLO QCD corrected differential cross section to the LO one (left) and to the (Born-improved) NLO HTL (right) for various definitions of the virtual top mass as a function of the invariant Higgs-pair mass M_{HH} for a c.m. energy $\sqrt{s} = 14$ TeV and using PDF4LHC parton densities.

independent) part $K_{\mathrm{SVC}}^{(i)}$ is dominant for the first few orders, while the moderate (top-mass dependent) remainder $K_{\mathrm{rem}}^{(i)}$ only adds 10–15% to the bulk of the corrections of ∼100%. The soft + virtual corrections $K_{\mathrm{SVC}}^{(i)}$ are basically the same for the (subleading) mass-effects at all orders, too. Since these pieces are part of the HTL at all perturbative orders, the Born-improved [3] and FTapprox [5] approaches provide a reasonable approximation of the total cross section within 10–15% at NLO. The mass effects at a given order are, thus, multiplied by the same universal correction factors, too. In the same way, the uncertainties originating from the mass effects are scaling with this dominant part of the QCD corrections. This statement is explicitly corroborated by the fact that the (Born-improved) HTL approximates the NLO cross section within about 15%, while the QCD corrections modify the cross section by close to 100%. Hence, at the state of the art, i.e., full NLO and NNLO[3] within the HTL with massive refinements, the best procedure to combine the *relative* uncertainties of Eqs. (5) and (6) is *linearly*. This will be not only the most conservative approach but close to the final numbers in a sophisticated combined calculation of the NNLO results in the HTL with the full NLO mass effects, i.e., with a negligible mismatch of the envelope from the linear combination.[4]

This procedure results in the following combined uncertainties of Eqs. (5) and (6),

$$\sqrt{s} = 13 \text{ TeV}: \sigma_{\mathrm{tot}} = 31.05^{+6\%}_{-23\%} \text{ fb,}$$
$$\sqrt{s} = 14 \text{ TeV}: \sigma_{\mathrm{tot}} = 36.69^{+6\%}_{-23\%} \text{ fb,}$$
$$\sqrt{s} = 27 \text{ TeV}: \sigma_{\mathrm{tot}} = 139.9^{+5\%}_{-22\%} \text{ fb,}$$
$$\sqrt{s} = 100 \text{ TeV}: \sigma_{\mathrm{tot}} = 1224^{+4\%}_{-21\%} \text{ fb.} \qquad (8)$$

The central values of these numbers have been obtained by using the top pole mass. In light of the findings of Refs. [8,16], the preferred scale choice is $\mu_t \sim M_{HH}$ at large values of M_{HH} so that the choice of the top pole mass for the central prediction can be questioned. However, for small values of M_{HH} close to the production threshold the process is quite close to the HTL, where the scale choice $\mu_t \sim m_t$ is the preferred one since the top mass constitutes the related matching scale. The scale choice $\mu_t = m_t$ is implicitly involved in the top pole mass, too. A further refinement of the proper scale choice for the virtual top mass would require an interpolation between the different kinematical regimes that would introduce a new uncertainty by itself. Such investigations are beyond the scope of this paper and all analyses so far. It should, however, be noted that the relative NLO top-mass effects turn out to be quite independent of M_{HH} if the top mass is defined as the $\overline{\mathrm{MS}}$ mass $\bar{m}_t(M_{HH}/4)$, as can be inferred from Fig. 1, where we display the ratio of the NLO cross section to the LO cross section[5] and to the Born-improved HTL at NLO (with the LO cross section determined in terms of the used top-mass definition) for various choices of the top mass. Adopting

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[3]In the future, the novel N[3]LO results will eventually become part of the recommended values.

[4]Our approach is not meant to estimate the uncertainties at full NNLO but the uncertainties at approximate NNLO without the knowledge of the complete m_t-effects at NNLO.

[5]It should be noted that the ratio to the LO cross section is not the consistently defined K factor. The latter requires the LO cross section to be evaluated with LO α_s and PDFs, while we use NLO quantities at LO, too, to show the pure effects of the matrix elements.

$\bar{m}_t(M_{HH}/4)$ for the top mass, the NLO mass effects range between 10% and 15% for the whole range in M_{HH} with a mild dependence on the invariant Higgs-pair mass, as can be inferred from the ratio to the HTL. The ratio to the LO cross section develops a very flat behavior for this scale choice, too.

IV. UNCERTAINTIES FOR DIFFERENT HIGGS SELF-INTERACTIONS

A variation of the trilinear Higgs coupling λ modifies the interplay between the LO box and triangle contributions that interfere destructively for the SM case. One of the basic questions is what will happen to the uncertainties for different values of λ. This can be traced back to the approximately aligned uncertainties of the triangle and box diagrams [8,18]. The renormalization and factorization scale uncertainties change by up to about 6% at NLO for large and small values of λ [17], such that the change with respect to the central uncertainties of the SM value of ∼10–15% is of moderate size. In a similar way the uncertainties originating from the scheme and scale choice of the top mass depend only mildly on the trilinear coupling λ. Equation (9) shows the central $\text{NNLO}_{\text{FTapprox}}$ predictions for the total cross section for various choices of $\kappa_\lambda = \lambda/\lambda_{\text{SM}}$ for $\sqrt{s} = 13$ TeV. The percent uncertainties display the usual factorization and renormalization scale uncertainties [19],

$$\kappa_\lambda = -10: \sigma_{\text{tot}} = 1680^{+3.0\%}_{-7.7\%} \text{ fb},$$
$$\kappa_\lambda = -5: \sigma_{\text{tot}} = 598.9^{+2.7\%}_{-7.5\%} \text{ fb},$$
$$\kappa_\lambda = -1: \sigma_{\text{tot}} = 131.9^{+2.5\%}_{-6.7\%} \text{ fb},$$
$$\kappa_\lambda = 0: \sigma_{\text{tot}} = 70.38^{+2.4\%}_{-6.1\%} \text{ fb},$$
$$\kappa_\lambda = 1: \sigma_{\text{tot}} = 31.05^{+2.2\%}_{-5.0\%} \text{ fb},$$
$$\kappa_\lambda = 2: \sigma_{\text{tot}} = 13.81^{+2.1\%}_{-4.9\%} \text{ fb},$$
$$\kappa_\lambda = 2.4: \sigma_{\text{tot}} = 13.10^{+2.3\%}_{-5.1\%} \text{ fb},$$
$$\kappa_\lambda = 3: \sigma_{\text{tot}} = 18.67^{+2.7\%}_{-7.3\%} \text{ fb},$$
$$\kappa_\lambda = 5: \sigma_{\text{tot}} = 94.82^{+4.9\%}_{-8.8\%} \text{ fb},$$
$$\kappa_\lambda = 10: \sigma_{\text{tot}} = 672.2^{+4.2\%}_{-8.5\%} \text{ fb}. \tag{9}$$

These predictions for the cross sections have been obtained by adopting the top pole mass for the LO and higher-order contributions. Modifying the scheme and scale choice of the top mass according to the SM analysis, we end up with the additional uncertainties at NLO,

$$\kappa_\lambda = -10: \sigma_{\text{tot}} = 1438(1)^{+10\%}_{-6\%} \text{ fb},$$
$$\kappa_\lambda = -5: \sigma_{\text{tot}} = 512.8(3)^{+10\%}_{-7\%} \text{ fb},$$
$$\kappa_\lambda = -1: \sigma_{\text{tot}} = 113.66(7)^{+8\%}_{-9\%} \text{ fb},$$
$$\kappa_\lambda = 0: \sigma_{\text{tot}} = 61.22(6)^{+6\%}_{-12\%} \text{ fb},$$
$$\kappa_\lambda = 1: \sigma_{\text{tot}} = 27.73(7)^{+4\%}_{-18\%} \text{ fb},$$

$$\kappa_\lambda = 2: \sigma_{\text{tot}} = 13.2(1)^{+1\%}_{-23\%} \text{ fb},$$
$$\kappa_\lambda = 2.4: \sigma_{\text{tot}} = 12.7(1)^{+4\%}_{-22\%} \text{ fb},$$
$$\kappa_\lambda = 3: \sigma_{\text{tot}} = 17.6(1)^{+9\%}_{-15\%} \text{ fb},$$
$$\kappa_\lambda = 5: \sigma_{\text{tot}} = 83.2(3)^{+13\%}_{-4\%} \text{ fb},$$
$$\kappa_\lambda = 10: \sigma_{\text{tot}} = 579(1)^{+12\%}_{-4\%} \text{ fb}. \tag{10}$$

The uncertainties originating from the scheme and scale choice of the top mass turn out to develop a mild dependence on κ_λ as expected. The size of the total uncertainty band is much less sensitive to κ_λ than the location of the band. Combining these relative uncertainties with the previous renormalization and factorization scale uncertainties of Eq. (9) *linearly*, we arrive at the central values with combined uncertainties,

$$\kappa_\lambda = -10: \sigma_{\text{tot}} = 1680^{+13\%}_{-14\%} \text{ fb},$$
$$\kappa_\lambda = -5: \sigma_{\text{tot}} = 598.9^{+13\%}_{-15\%} \text{ fb},$$
$$\kappa_\lambda = -1: \sigma_{\text{tot}} = 131.9^{+11\%}_{-16\%} \text{ fb},$$
$$\kappa_\lambda = 0: \sigma_{\text{tot}} = 70.38^{+8\%}_{-18\%} \text{ fb},$$
$$\kappa_\lambda = 1: \sigma_{\text{tot}} = 31.05^{+6\%}_{-23\%} \text{ fb},$$
$$\kappa_\lambda = 2: \sigma_{\text{tot}} = 13.81^{+3\%}_{-28\%} \text{ fb},$$
$$\kappa_\lambda = 2.4: \sigma_{\text{tot}} = 13.10^{+6\%}_{-27\%} \text{ fb},$$
$$\kappa_\lambda = 3: \sigma_{\text{tot}} = 18.67^{+12\%}_{-22\%} \text{ fb},$$
$$\kappa_\lambda = 5: \sigma_{\text{tot}} = 94.82^{+18\%}_{-13\%} \text{ fb},$$
$$\kappa_\lambda = 10: \sigma_{\text{tot}} = 672.2^{+16\%}_{-13\%} \text{ fb}. \tag{11}$$

These final numbers should serve as the recommended values for the total cross sections and uncertainties at the LHC with $\sqrt{s} = 13$ TeV as a function of κ_λ.

V. CONCLUSIONS

We have analyzed the combination of the usual renormalization and factorization scale uncertainties of Higgs-pair production via gluon fusion with the uncertainties originating from the scheme and scale choice of the virtual top mass in the Yukawa coupling and the propagators. Due to the observation that the latter relative uncertainties are nearly independent of the renormalization and factorization scale choices, the proper combination of the relative uncertainties is provided by a linear addition. Our procedure does not estimate the full uncertainties at NNLO but those at approximate NNLO without the knowledge of the complete NNLO top-mass effects.

In a second step we derived the dependence of the uncertainties related to the top-mass scheme and scale choice on a variation of the trilinear Higgs self-coupling λ. The relative uncertainties are again observed to develop only a small dependence on λ. We combined all the

uncertainties for $\sqrt{s} = 13$ TeV with the ones of the present recommendation of the LHC Higgs Working Group, obtaining state-of-the-art predictions for Higgs pair production cross sections at the LHC, including both renormalization/factorization scale and top-quark scale and scheme uncertainties.

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