

Next-to-next-to-leading order event generation for Z-boson production in association with a bottom-quark pair

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We consider the production of a Z boson decaying to leptons in association with a bottom-quark pair in hadronic collisions. For the first time, we compute predictions at next-to-next-to-leading order (NNLO) in QCD, and we combine them with the all-order radiative corrections from a parton-shower simulation (NNLO + PS). Our method represents the first approach to NNLO + PS event generation applicable to processes featuring a color singlet and a heavy-quark pair in the final state. The novel two-loop corrections are computed for massless bottom quarks, and the leading mass corrections are restored through a small-mass expansion. The calculation is carried out in the four-flavor scheme, and we find that the sizable NNLO QCD corrections lift the long-standing tension between lower-order predictions in four- and five-flavor schemes. Our predictions are compared to a CMS measurement for Z boson plus b -jet production, achieving an excellent description of the data.

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I. INTRODUCTION

The quest to uncover signals of new physics at the Large Hadron Collider (LHC) has become a major endeavor within the extensive physics program of the LHC experiments, encompassing both the direct detection of resonances and the analysis of small deviations from the Standard Model (SM) through precision measurements. The success of the latter critically depends on the availability of highly accurate simulations and predictions for all classes of LHC reactions.

The associated production of a Z boson and a bottom-quark pair ($b\bar{b}Z$) plays a special role in the LHC physics program. For one, it yields heavy-quark mass effects to Drell-Yan production, a process that is measured very accurately at hadron colliders and used to extract the mass of the W boson; see, e.g., Refs. [1–3]. Moreover, $b\bar{b}Z$ production is a major background to ZH measurements [4,5] and to various beyond the SM searches; see, e.g., Ref. [6].

Precision measurements of Z-boson production with bottom-flavored jets (b jets) have been performed both at the Tevatron [7–9] and by the LHC experiments [10–17]. So far, there has been a significant discrepancy among the

$Z + b$ -jet theory predictions, depending on whether the bottom quark is assumed to be massive in a four-flavor scheme (4FS) or massless in a five-flavor scheme (5FS) calculation [18]. Especially, state-of-the-art 4FS predictions are in tension with measurements of $Z + b$ -jet production [10,11,13,14,18].

Next-to-leading order (NLO) corrections in QCD have been computed both in the 4FS [19] (see also Ref. [20]) and in the 5FS [21]. In the 5FS, Z-boson production with a single b jet is known through next-to-next-to-leading order (NNLO) [22]. References [19,23] showed that the inclusion of bottom-mass effects in the 4FS is important for the $b\bar{b}Z$ cross section and in kinematic distributions of the bottom quarks for scales close to m_b . The matching of the NLO corrections with a parton shower (NLO + PS) is available in both schemes within MadGraph5_aMC@NLO [24] and within Sherpa [18], where the 5FS implementation in Sherpa includes up to two extra b jets at NLO + PS via multijet merging. The combination of four- and five-flavor predictions at NLO + PS was achieved in Ref. [25]; see also Ref. [26] for an earlier study. Higher-order corrections to $b\bar{b}Z$ production are substantial, especially in the 4FS, with very sizable perturbative uncertainties. Prior to this work, no NNLO results had been obtained for any of the flavor schemes.

In this paper, we considerably improve the accuracy of $Z + b$ -jet theory predictions by computing the NNLO QCD corrections to $b\bar{b}Z$ production for massive bottom quarks. Our results are implemented in a fully exclusive Monte Carlo event generator by matching the NNLO

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corrections to a parton shower (NNLO + PS). Our approach represents the first NNLO + PS method for such an involved final state, featuring both a heavy-quark pair and a set of color-singlet particles. The two-loop corrections for the $b\bar{b}Z$ process are presented here for the first time, by exploiting the massless amplitudes [27] to approximate the massive ones. We use our novel results to investigate whether the NNLO corrections resolve the long-standing discrepancies between 4FS and 5FS predictions and compare our results with the latest $Z + b$ -jet measurement by CMS [15] to assess their impact on the tension of previous 4FS predictions with LHC data.

II. METHODOLOGY

We consider the process

$$pp \rightarrow b\bar{b}\ell^+\ell^- + X, \quad (1)$$

which we denote as $b\bar{b}Z$ production for brevity. Sample Feynman diagrams at the leading order (LO) are shown in Fig. 1. They involve both quark- and gluon-initiated channels, where the Z boson can be radiated off any of the quark lines.

Among the NNLO + PS frameworks for color-singlet production [28–32], only the MiNNLO_{PS} approach [31,32] has been extended to processes featuring color charges in initial and final states, namely, heavy-quark pair production [33–35]. We further extend the MiNNLO_{PS} method to construct a fully exclusive NNLO + PS generator for the associated production of a heavy-quark pair ($Q\bar{Q}$) with system color-singlet particles (F).

The general structure of large logarithmic contributions at small transverse momentum for $Q\bar{Q}$ and $Q\bar{Q}F$ production is very similar [36]. As a result, we can exploit the analytic formula for the cross section differential in the transverse momentum $p_T \equiv |\vec{p}_T|$ and the Born phase space Φ_B of the final-state system, which was derived in Refs. [33,34] from the well-known factorization theorem for $Q\bar{Q}$ production at small p_T [37–40] and can be written symbolically as

$$\frac{d\sigma}{dp_T d\Phi_B} = \frac{d}{dp_T} \left\{ \sum_c \left[\sum_{i=1}^{n_c} \mathcal{C}_{c\bar{c}}^{[y_i]} e^{-\tilde{S}_{c\bar{c}}^{[y_i]}} \right] \mathcal{L}_{c\bar{c}} \right\} + R_f. \quad (2)$$

The first term includes the singular (and constant) contributions in p_T , which represents the transverse

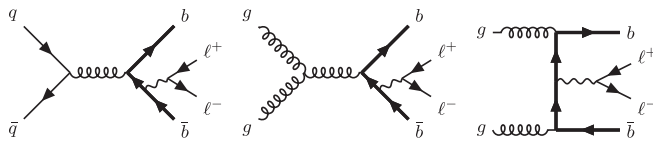


FIG. 1. Feynman diagrams for $pp \rightarrow b\bar{b}\ell^+\ell^-$ at LO.

momentum of the $Q\bar{Q}F$ system here, while R_f adds the regular contributions.

This formula retains NNLO plus leading-logarithmic accuracy, and it preserves the class of next-to-leading-logarithmic corrections that traditional PS algorithms [41] include. Therefore, it is the starting point to build a Monte Carlo algorithm for the generation of NNLO events within the POWHEG framework [42,43], which has been demonstrated several times [31,32,34], most recently for $Q\bar{Q}$ production in Ref. [34]. In the following, instead, we focus on the main changes from $Q\bar{Q}$ to $Q\bar{Q}F$ processes.

The sum over c in Eq. (2) runs over the flavor configurations $\{g, q, \bar{q}\}$ of the incoming partons. On the other hand, the sum over i originates from diagonalizing the one-loop soft anomalous dimension $\mathbf{\Gamma}^{(1)}$ with complex coefficients $\mathcal{C}_{c\bar{c}}^{[y_i]}$ that fulfill $\sum_{i=1}^{n_c} \mathcal{C}_i = 1$, where n_c is determined by the SU(3) representation of a given flavor configuration.¹ The eigenvalues of $\mathbf{\Gamma}^{(1)}$, denoted by γ_i , induce a modification to the Sudakov exponent, as indicated by the notation $\tilde{S}^{[y_i]}$. We note that $\mathbf{\Gamma}^{(1)}$, γ_i , and $\mathcal{C}_{c\bar{c}}^{[y_i]}$ have the same form as for $Q\bar{Q}$ production (see Appendix A of Ref. [34]) except for adapting the process-dependent LO matrix element in the definition of $\mathcal{C}_{c\bar{c}}^{[y_i]}$. We construct this matrix element from color-decomposed scattering amplitudes of OpenLoops [44–46]. Contributions from $\mathbf{\Gamma}^{(2)}$ are included in the Sudakov exponent with an approximation of its corrections beyond NNLO. The general form of $\mathbf{\Gamma}^{(2)}$ includes terms proportional to three parton correlations, whose expectation value with the LO matrix element vanishes in the $Q\bar{Q}$ case. For $Q\bar{Q}F$ processes they contribute; therefore, we include them in our implementation.

The factor $\mathcal{L}_{c\bar{c}}$ in Eq. (2) includes the squared matrix elements for $Q\bar{Q}F$ production, encoded in the hard-virtual function $H_{c\bar{c}}$ defined below, and the convolution of the collinear coefficient functions with the parton distribution functions (PDFs). For the gluon-initiated channel, $\mathcal{L}_{c\bar{c}}$ features azimuthal-angle correlations, which originate from initial-state collinear emissions [47] and from soft emissions connecting all the hard partons in the process [39]. Starting at NNLO, these contributions give a nonvanishing contribution even after performing the azimuthal average over $\vec{p}_T$. For the case of $Q\bar{Q}$ production, they were computed analytically in Ref. [48]. For $Q\bar{Q}F$ processes, we compute them through a numerical integration over the azimuthal angle in conjugate space (b space). We note that the explicit azimuthal dependence plays a role only beyond the logarithmic accuracy in which we are interested.

The hard-virtual function is defined as

$$H_{c\bar{c}} = \frac{\langle \mathcal{R}_{c\bar{c}} | \bar{\mathbf{h}}^\dagger \mathbf{h} | \mathcal{R}_{c\bar{c}} \rangle}{\langle \mathcal{R}_{c\bar{c}}^{(0)} | \mathcal{R}_{c\bar{c}}^{(0)} \rangle}, \quad \bar{\mathbf{h}} | \mathcal{R}_{c\bar{c}} \rangle = \bar{\mathbf{h}} \mathbf{Z}^{-1} | \mathcal{M}_{c\bar{c}} \rangle, \quad (3)$$

¹The notation $X^{(i)}$ denotes the i th term in the perturbative expansion of the quantity X with respect to $\alpha_s/(2\pi)$.

where $\mathcal{R}_{c\bar{c}}$ is the finite remainder obtained from the virtual amplitude $\mathcal{M}_{c\bar{c}}$ after removing the IR divergences through the operator $\mathbf{Z}^{-1}$ [49,50], $\langle \mathcal{R}_{c\bar{c}}^{(0)} | \mathcal{R}_{c\bar{c}}^{(0)} \rangle = |M_{c\bar{c}}^{(0)}|^2$, and the operator $\mathbf{h}$ determines parton emissions of soft origin, which are known for $Q\bar{Q}$ production up to NNLO [51]. Here, we employ their extension to the general kinematics of $Q\bar{Q}F$ production [52].

The process-dependent pieces entering the hard function are the finite remainders up to two loops. We obtain the one-loop amplitude entering $H_{c\bar{c}}^{(1)}$ and one-loop squared amplitude entering $H_{c\bar{c}}^{(2)}$ from OpenLoops. While all other contributions are taken exactly, we calculate the two-loop finite remainder $2\text{Re}\langle \mathcal{R}_{c\bar{c}}^{(0)} | \mathcal{R}_{c\bar{c}}^{(2)} \rangle$ entering $H_{c\bar{c}}^{(2)}$ in an approximation, since its full computation is well beyond current technology for two-loop, five-point amplitudes. Realizing that there is a hierarchy in the bottom-quark mass m_b , we can perform an expansion around small m_b of the two-loop amplitude, capturing the constant and logarithmically enhanced terms in m_b , while omitting power corrections in m_b ,

$$\frac{2\text{Re}\langle \mathcal{R}_{c\bar{c}}^{(0)} | \mathcal{R}_{c\bar{c}}^{(2)} \rangle}{\langle \mathcal{R}_{c\bar{c}}^{(0)} | \mathcal{R}_{c\bar{c}}^{(0)} \rangle} = \frac{2\text{Re}\langle \mathcal{R}_{0,c\bar{c}}^{(0)} | \mathcal{R}_{0,c\bar{c}}^{(2)} \rangle}{\langle \mathcal{R}_{0,c\bar{c}}^{(0)} | \mathcal{R}_{0,c\bar{c}}^{(0)} \rangle} + \sum_{i=0}^4 \kappa_{c\bar{c},i} \log\left(\frac{m_b}{\mu_R}\right)^i + \mathcal{O}\left(\frac{m_b}{\mu_h}\right), \quad (4)$$

where $\mathcal{R}_{0,c\bar{c}}^{(i)}$ denotes the finite remainder of the “massless” $b\bar{b}Z$ amplitude, i.e., setting $m_b = 0$, μ_R is the renormalization scale, and μ_h is a characteristic hard scale of the process. The process-dependent coefficients $\kappa_{c\bar{c},i}$ are determined in Appendix A. They are obtained through a “massification” procedure that relates the $1/\epsilon^i$ poles of collinear origin in the 5FS with logarithmic terms in m_b in the 4FS [53,54]; see also Ref. [55] for a recent application to $b\bar{b}W$ production.

In the massless case, the calculation of the two-loop amplitude is still very challenging, but feasible [27]. While the logarithmic terms are reproduced without any approximations, $\text{Re}\langle \mathcal{R}_{0,c\bar{c}}^{(0)} | \mathcal{R}_{0,c\bar{c}}^{(2)} \rangle$ is computed in the leading-color approximation (LCA), with the exception of contributions of Z/γ^* bosons coupling to closed fermion loops, which are omitted. We have tested the latter to be negligible already at the one-loop level (see also Refs. [56,57]). The LCA is typically accurate within 10% (see, e.g., Refs. [58,59]). Since the numerical effect of $\langle \mathcal{R}_{0,c\bar{c}}^{(0)} | \mathcal{R}_{0,c\bar{c}}^{(2)} \rangle$ on the MiNNLO_{PS} cross section is typically at the few-percent level, we expect these approximations to have a negligible impact on our results. To calculate $\text{Re}\langle \mathcal{R}_{0,c\bar{c}}^{(0)} | \mathcal{R}_{0,c\bar{c}}^{(2)} \rangle$, we have implemented a numerical code based on the analytic results of Ref. [27], employing the

PentagonFunctions++ code [60–62] to evaluate the relevant special functions.

We note that our calculation of the logarithmically enhanced terms in Eq. (4) has been rendered possible for closed massive fermion loops only by the recent results of Ref. [54]. However, the numerical impact of those contributions turns out to be tiny, at the few-permille level of the NNLO cross section, which we have tested both by excluding them from the two-loop finite remainder and by turning top and bottom loops off in the rest of the calculation.

Since our NNLO + PS generator assumes massive bottom quarks, a mapping from the massive to the massless phase space is required to evaluate the massless remainders $\mathcal{R}_{0,c\bar{c}}^{(i)}$. While different mappings induce only power corrections in m_b/μ_h , it is mandatory that the mapping avoids the collinear singularities of the massless amplitudes, which in the massive phase space are prevented by the bottom mass.² We have tested different mappings and found their results to agree at the subpercent level. The details are given in Appendix B.

III. RESULTS

For the phenomenological study of $b\bar{b}Z$ production at NNLO + PS, we focus on LHC collisions with 13 TeV center-of-mass energy and consider the leptonic final states with $\ell = e, \mu$. The bottom- and top-quark on-shell masses are set to 4.92 and 173.2 GeV, respectively, with four massless quark flavors. We employ the corresponding NNLO set of the NNPDF31 [63] parton densities with $\alpha_s(m_Z) = 0.118$. We use the complex-mass scheme [64,65] and the electroweak input parameters are set in the G_μ scheme using [66]: $G_F = 1.16639 \times 10^{-5} \text{ GeV}^{-2}$ and $M_W = 80.385$, $\Gamma_W = 2.0854$, $m_Z = 91.1876$, and $\Gamma_Z = 2.4952 \text{ GeV}$. Unless specified otherwise, our default choice for the renormalization scale of the two powers of the α_s at Born level is $\mu_R^{(0)} = m_{b\bar{b}\ell\ell}$. The scale of extra powers of α_s in the radiative corrections and the factorization scale are set following the MiNNLO_{PS} prescription [31,34]. We employ the definition of the modified logarithm L in Ref. [34], which smoothly turns off resummation effects for p_T values larger than $Q = m_{b\bar{b}\ell\ell}/2$. To avoid the Landau singularity at small p_T , the scale of the strong coupling and the parton densities is smoothly frozen around $Q_0 = 2 \text{ GeV}$ [32]. Scale uncertainties are estimated through the usual seven-point scale variations by a factor of 2 around the central scale. As a parton shower, we employ Pythia8 [67] with the Monash tune [68].

For comparison, we implemented a generator for $pp \rightarrow b\bar{b}\ell^+\ell^-$ production at NLO + PS in the 4FS within POWHEG-BOX-RES [43]. In this case, we use $m_{b\bar{b}\ell\ell}$ for

²We thank Chiara Savoini and Massimiliano Grazzini for bringing this to our attention.

TABLE I. Total $b\bar{b}Z$ cross section with $66 \leq m_{\ell^+\ell^-} \leq 116$ GeV. The scale in brackets indicates the different scale setting as described in the text. The quoted errors represent scale uncertainties, while the numbers in brackets are numerical uncertainties on the last digit.

	σ_{total} (pb)	Ratio to NLO
NLO + PS ($m_{b\bar{b}\ell\ell}$)	31.86(1) $^{+16.3\%}_{-13.3\%}$	1.000
MiNLO' ($m_{b\bar{b}\ell\ell}$)	22.33(1) $^{+28.2\%}_{-17.9\%}$	0.701
MiNNLO _{PS} ($m_{b\bar{b}\ell\ell}$)	50.17(4) $^{+16.5\%}_{-12.0\%}$	1.575
NLO + PS ($H_T/2$)	41.42(1) $^{+19.2\%}_{-15.4\%}$	1.000
MiNNLO _{PS} ($H_T/2$)	57.09(4) $^{+17.8\%}_{-12.7\%}$	1.378

the central scales. We also evaluate MiNLO' results, which are NLO accurate for $b\bar{b}\ell^+\ell^-$ plus zero and one jet, by turning off the NNLO corrections in the MiNNLO_{PS} generator.

Table I shows the $pp \rightarrow b\bar{b}\ell^+\ell^-$ total cross section. For reference, NLO + PS (MiNNLO_{PS}) results with a central scale $H_T/2$ [$\mu_R^{(0)} = H_T/2$] are given as well, where H_T is the sum over the transverse masses of each bottom quark and each lepton. Shower effects are negligible for the inclusive rate and, only for the results presented in this table, we have turned off the effects of hadronization, multiparton interactions (MPIs), and QED radiation.

The MiNLO' prediction, which is formally NLO accurate and includes additional $\mathcal{O}(\alpha_s^2)$ corrections, is 43% smaller than the other NLO + PS result and does not provide a reasonable prediction. Although this may seem surprising, this behavior can be explained by the substantial cancellation of logarithmic corrections in m_b between the real (double-real and real-virtual) and the double-virtual amplitudes. Those logarithmic terms originate from the massive bottom quark in the 4FS, which regulates the real phase-space integration as well as the loop integration. The ensuing logarithmic contributions are bound to cancel between real- and double-virtual amplitudes, which can be understood by considering the 5FS, where these logarithms would appear as $1/\epsilon$ poles that cancel by the Kinoshita-Lee-Nauenberg theorem [69,70].

For MiNLO', the relative $\mathcal{O}(\alpha_s^2)$ contribution is incomplete, as only the real amplitudes are included and the corresponding logarithmic terms induce a numerically significant negative effect. We have checked that it is sufficient to include the dominant logarithmic corrections in the double-virtual amplitudes (obtained using the massification procedure in Appendix A) to restore the appropriate cancellation and obtain a positive $\mathcal{O}(\alpha_s^2)$ correction. Because of this unphysical effect, we refrain from including MiNLO' results in the remainder of this paper.

Considering the MiNNLO_{PS} predictions in Table I, NNLO corrections increase the NLO cross section by 57%, which renders them crucial for an accurate prediction in

TABLE II. Comparison of theory predictions with the fiducial cross section measurements by CMS [15] for (at least) one and two tagged b jets. Experimental uncertainties are added in quadrature. The 5FS result is taken from Ref. [15] and scale uncertainties have been symmetrized by taking the maximum of the absolute value of the errors.

σ_{fiducial} (pb)	$Z + \geq 1$ b jet	$Z + \geq 2$ b jets
NLO + PS (5FS) [15]	7.03 ± 0.47	0.77 ± 0.07
NLO + PS (4FS)	4.08 ± 0.66	0.44 ± 0.08
MiNNLO _{PS} (4FS)	6.62 ± 0.86	0.76 ± 0.09
CMS [15]	6.52 ± 0.43	0.65 ± 0.08

the 4FS. Since the NNLO corrections are much larger than the NLO scale uncertainties, we consider $H_T/2$ as a second scale choice. In this case, the NLO and the NNLO cross sections are larger, with NNLO corrections of about 38%. While the NNLO scale uncertainties are still very sizable, as expected for a process featuring very large perturbative corrections, it is reassuring that the dependence on the scale choice reduces at NNLO compared to NLO.

In Table II, we consider the fiducial cross section measurement of the most recent CMS analysis for Z -boson production in association with bottom-flavored jets [15], which includes the complete Run-2 dataset of the LHC. The fiducial cuts are defined in Appendix C. To warrant a realistic comparison to data, we include effects from hadronization, MPIs, and QED radiation from now on. In our 4FS calculation, we can directly apply the experimental definition of b jets, which is rendered infrared safe by the bottom mass, while in the 5FS, the naive definition of b jets leads to divergences [71–75]. For the $Z + \geq 1(2)$ b -jet rate, we observe a clear tension with the NLO + PS result in the 4FS, whose central cross section is 40(20)% below the measurement, well outside the uncertainties. By contrast, the MiNNLO_{PS} prediction is in agreement with the data within uncertainties.

In addition, we include in Table II the NLO + PS prediction in the 5FS, as quoted in the CMS analysis [15] and obtained with MadGraph5_aMC@NLO [76].³ NLO + PS results in the 4FS and 5FS are not compatible with each other, but our MiNNLO_{PS} prediction agrees with the 5FS result, thanks to the inclusion of NNLO QCD corrections in the 4FS. We note that the larger scale uncertainties observed in the 4FS are related to its slower perturbative convergence, which is apparent from the much larger higher-order corrections compared to the 5FS. While the predictions in both schemes agree similarly well with the $Z + \geq 2b$ -jet data, MiNNLO_{PS} shows a better description in the $Z + \geq 1b$ -jet fiducial region.

³We note that several NLO + PS predictions are quoted in Ref. [15]. The one quoted in Table II is the only one using the same PDF set as in our setup.

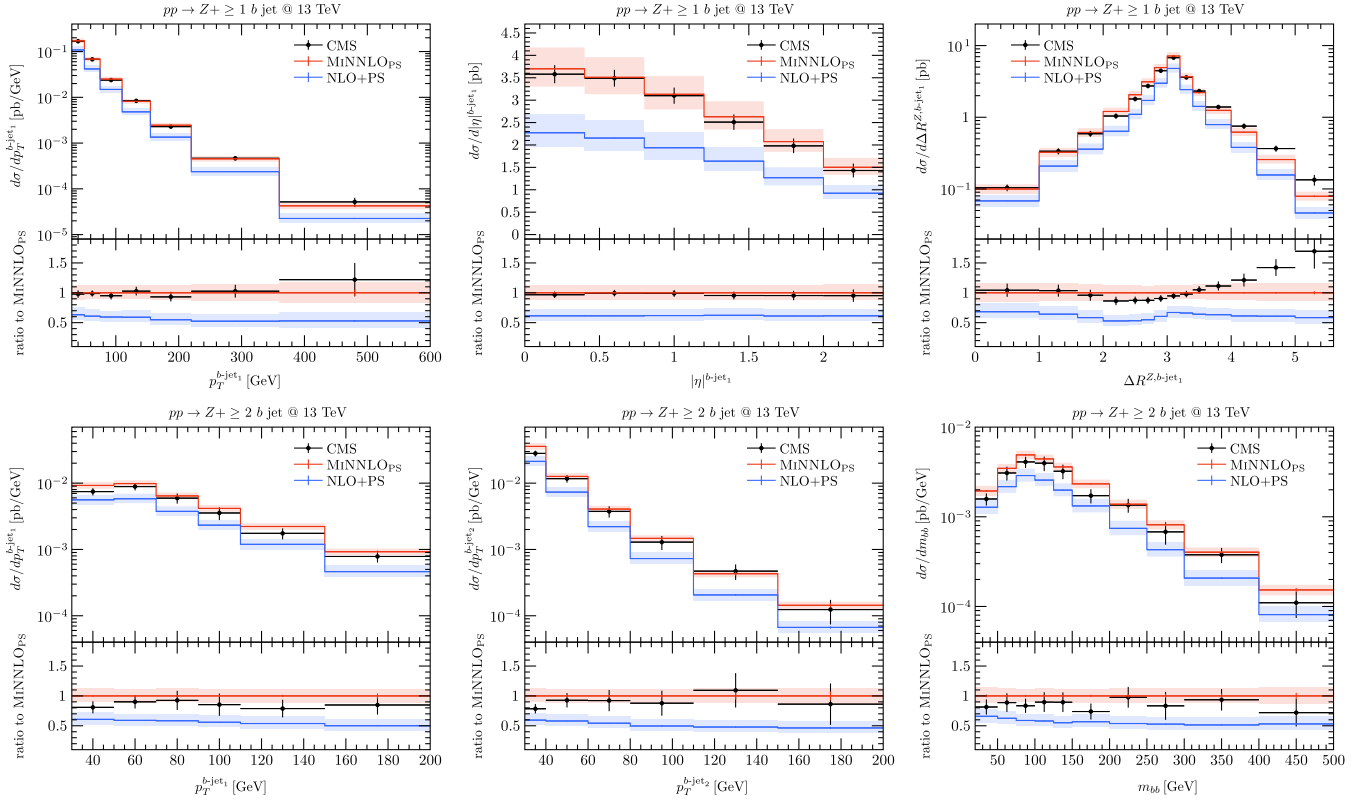


FIG. 2. Comparison of theory predictions with differential distributions measured by CMS [15].

Next, we examine a set of differential distributions in Fig. 2 and compare NLO + PS (blue, dashed) and MiNNLO_{PS} (red, solid) predictions to the CMS measurement (black data points) [15]. The upper three panels show the inclusive one b -jet phase space: the transverse momentum ($p_T^{b\text{-jet}_1}$) and pseudorapidity ($|\eta|^{b\text{-jet}_1}$) of the leading b jet as well as the distance between the Z boson and the leading b jet in the $\eta - \phi$ plane ($\Delta R^{Z,b\text{-jet}_1}$). The lower three panels show distributions in the inclusive two b -jet phase space: the transverse momentum of the leading ($p_T^{b\text{-jet}_1}$) and subleading b jet ($p_T^{b\text{-jet}_2}$), as well as the invariant mass of the two b jets (m_{bb}).

As observed for the fiducial rates, NLO + PS predictions fail in describing the normalization of the measured cross sections. Additionally, the shapes of some of the distributions are not reproduced particularly well. The MiNNLO_{PS} predictions, on the other hand, are in agreement with data, especially for $Z + \geq 1$ b -jet observables the central prediction is almost spot on the data points, which is remarkable considering the relatively high precision of theory predictions and measurement. In the inclusive two b -jet phase space, the experimental errors are larger due to the lower statistics. Here, MiNNLO_{PS} predicts a normalization slightly higher than the data points, but still fully covered by the uncertainties, while the differential shapes are reproduced particularly well.

An exception to the previous statements about MiNNLO_{PS} is the difference observed at high $\Delta R^{Z,b\text{-jet}_1}$ with the CMS data, which originate from large values of the rapidity separation between the Z boson and the leading b jet ($\Delta y^{Z,b\text{-jet}_1}$), where similar differences appear. Although less pronounced than in the 4FS, such trend is also present in the 5FS predictions at large $\Delta y^{Z,b\text{-jet}_1}$ and $\Delta R^{Z,b\text{-jet}_1}$; see Figs. 6 and 7 of Ref. [15]. That behavior also appears in the $\Delta y^{Z,b\text{-jet}_1}$ distribution in an earlier ATLAS measurement [14]. A better understanding of this discrepancy requires additional studies and potentially all-order resummation of logarithms in m_b through a 4FS and 5FS combination at NNLO + PS, which is left for future work.

IV. SUMMARY

In this paper, we presented a novel computation for the production of a Z boson in association with bottom quarks in hadronic collisions. We have calculated NNLO QCD corrections in the 4FS, including the five-point, two-loop amplitude in the small- m_b approximation. In addition, the first NNLO + PS approach for the production of a heavy-quark pair in association with color-singlet particles has been developed, which can be readily applied to other processes, like $b\bar{b}W$ [55], $t\bar{t}W$ [77], and $t\bar{t}H$ [78] production.

Our NNLO + PS calculation solves two (related) long-standing issues for $b\bar{b}Z$ production: First, the significant

tension of NLO(+PS) predictions in the 4FS with experimental data and, second, the large differences between 4FS and 5FS predictions for this process [18]. Our analysis identifies that missing higher-order corrections in the 4FS cause these discrepancies and that the perturbative accuracy of previous calculations has been insufficient. Including NNLO QCD corrections brings the 4FS predictions in agreement with the experimental data and with the 5FS results. The calculation presented in this paper also builds the basis for a more accurate determination of the bottom-quark mass effects in Drell-Yan production, relevant for M_W measurements, along the lines of the study in Ref. [79], which at the time was pursued only at NLO + PS.

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massification procedure with us, and we thank Chiara Savoini and Massimiliano Grazzini for bringing to our attention the issues related to the singular behavior of the massless amplitudes for certain mappings from the massive to the massless momenta of the bottom quarks. V. S. has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme Grant agreement 101019620 (ERC Advanced Grant TOPUP).

APPENDIX A: FINITE MASSIFICATION

In this appendix, we provide additional details on the small bottom-mass approximation (exploiting a massification procedure) that we use to compute the two-loop amplitude for $b\bar{b}Z$ production. The massification procedure allows us to approximate a massive amplitude from the massless one, while dropping power corrections in the bottom mass m_b , but reproducing correctly all logarithmic terms in m_b .

We aim to calculate the finite remainder $|\mathcal{R}\rangle = \mathbf{Z}^{-1}|\mathcal{M}\rangle$ defined in Eq. (3) (we leave the channel labels implicit for clarity of the formulas) in the small bottom-mass approximation. Using the factorization formula from Refs. [53,54], we obtain

$$|\mathcal{R}_{m_b \ll \mu_h}\rangle = \mathbf{Z}_{m_b \ll \mu_h}^{-1} \mathcal{F} \mathbf{S} \mathbf{Z}_0 |\mathcal{R}_0\rangle \Big|_{n_f=n_l+n_h}, \quad \text{with} \quad |\mathcal{R}\rangle = |\mathcal{R}_{m_b \ll \mu_h}\rangle + \mathcal{O}\left(\frac{m_b}{\mu_h}\right), \quad (\text{A1})$$

where μ_h is the characteristic hard scale of the process, $|\mathcal{R}_0\rangle = \mathbf{Z}_0^{-1}|\mathcal{M}_0\rangle$ is the massless finite remainder defined through the massless IR renormalization operator $\mathbf{Z}_0$ [49,50], and $\mathbf{Z}_{m_b \ll \mu_h}$ is the small-mass expansion of $\mathbf{Z}$. The channel-dependent operators $\mathcal{F}$ are defined as

$$\mathcal{F}_{q\bar{q}} = \mathcal{Z}_{[Q]} \mathcal{Z}_{[q]}, \quad \mathcal{F}_{gg} = \mathcal{Z}_{[g]} \mathcal{Z}_{[q]}, \quad (\text{A2})$$

with the functions $\mathcal{Z}_{[i]}$ given in Refs. [53,54], and $\mathbf{S}$ is the soft function introduced in Ref. [54] that is required to approximate contributions from heavy-quark loops. Here $\mathbf{Z}_0$ and $|\mathcal{R}_0\rangle$ depend on the total number of flavors

$n_f = n_l + n_h$, which is determined by the number of $n_l = 4$ light flavors in the 4FS and $n_h = 1$ heavy flavors corresponding to the bottom quark. Since the top quark practically decouples due to its large mass, its loop corrections are expected to be negligible. Therefore, we discard contributions from top loops here.

We introduce functions $\bar{\mathcal{F}}$ and $\bar{\mathbf{S}}$ free from ϵ poles, such that $\bar{\mathcal{F}} \bar{\mathbf{S}} = \mathbf{Z}_{m_b \ll \mu_h}^{-1} \mathcal{F} \mathbf{S} \mathbf{Z}_0$. Here, $\bar{\mathcal{F}}$ is diagonal in color space, while $\bar{\mathbf{S}}$ is a matrix in color space. We start by writing their perturbative expansions in the strong coupling constant $\alpha_s^{n_f}$, which includes the heavy flavors in its running,

$$\bar{\mathcal{F}} = 1 + \left(\frac{\alpha_s^{n_f}}{2\pi}\right) \bar{\mathcal{F}}^{(1)} + \left(\frac{\alpha_s^{n_f}}{2\pi}\right)^2 \bar{\mathcal{F}}^{(2)} + \mathcal{O}(\alpha_s^3), \quad (\text{A3})$$

$$\bar{\mathbf{S}} = 1 + \left(\frac{\alpha_s^{n_f}}{2\pi}\right)^2 \mathbf{C}_d \mathcal{S}^{(2)} + \mathcal{O}(\alpha_s^3), \quad \mathbf{C}_d = \sum_{(i,j)} -\frac{\mathbf{T}_i \cdot \mathbf{T}_j}{2} \log\left(\frac{-s_{ij}}{\mu_R^2}\right), \quad (\text{A4})$$

where $\mathbf{C}_d$ is the standard dipole color-space operator (see, e.g., Ref. [50]), and the coefficients are

$$\bar{\mathcal{F}}^{(1)} = 2C_F \ell_b^2 + C_F \ell_b + C_F \left(2 + \frac{\pi^2}{12}\right) + n_h \bar{\mathcal{F}}_{n_h, c\bar{c}}^{(1)}, \quad \text{with} \quad \bar{\mathcal{F}}_{n_h, q\bar{q}}^{(1)} = 0, \quad \bar{\mathcal{F}}_{n_h, gg}^{(1)} = -\frac{2}{3} \ell_b, \quad (\text{A5})$$

$$\begin{aligned}
\bar{\mathcal{F}}^{(2)} = & 2C_F^2\ell_b^4 + \ell_b^3 \left(\frac{22}{9}C_AC_F + 2C_F^2 - \frac{4}{9}C_Fn_l \right) + \ell_b^2 \left(C_AC_F \left(\frac{167}{18} - \frac{\pi^2}{3} \right) + C_F^2 \left(\frac{9}{2} + \frac{\pi^2}{6} \right) - \frac{13}{9}C_Fn_l \right) \\
& + \ell_b \left(C_AC_F \left(\frac{1165}{108} + \frac{14}{9}\pi^2 - 15\zeta_3 \right) + C_F^2 \left(\frac{11}{4} - \frac{11}{12}\pi^2 + 12\zeta_3 \right) - C_Fn_l \left(\frac{77}{54} + \frac{2}{9}\pi^2 \right) \right) \\
& + C_F^2 \left(\frac{241}{32} - \frac{163}{1440}\pi^4 + \pi^2 \left(\frac{13}{12} - 2\log(2) \right) - \frac{3}{2}\zeta_3 \right) + C_AC_F \left(\frac{12877}{2592} - \frac{47}{720}\pi^4 + \pi^2 \left(\frac{323}{432} + \log(2) \right) + \frac{89}{36}\zeta_3 \right) \\
& - C_Fn_l \left(\frac{1541}{1296} + \frac{37}{216}\pi^2 + \frac{13}{18}\zeta_3 \right) + n_h \bar{\mathcal{F}}_{n_h, c\bar{c}}^{(2)}, \tag{A6}
\end{aligned}$$

with

$$\bar{\mathcal{F}}_{n_h, q\bar{q}}^{(2)} = -\frac{20}{9}\ell_b^3C_F + \frac{32}{9}\ell_b^2C_F + \ell_bC_F \left(-\frac{157}{27} - \frac{7}{18}\pi^2 \right) + C_F \left(\frac{1933}{324} - \frac{13}{108}\pi^2 - \frac{7}{9}\zeta_3 \right), \tag{A7}$$

$$\begin{aligned}
\bar{\mathcal{F}}_{n_h, gg}^{(2)} = & \ell_b^3 \left(-\frac{4}{9}C_A - \frac{28}{9}C_F \right) + \ell_b^2 \left(\frac{10}{9}C_A + \frac{7}{9}C_F \right) + \ell_b \left(C_F \left(-\frac{319}{54} - \frac{5}{18}\pi^2 \right) + C_A \left(-\frac{92}{27} + \frac{\pi^2}{18} \right) \right) \\
& + C_A \left(\frac{179}{108} - \frac{5}{216}\pi^2 - \frac{7}{18}\zeta_3 \right) + C_F \left(\frac{2677}{1296} - \frac{41}{216}\pi^2 - \frac{\zeta_3}{18} \right) + \frac{4}{9}n_h\ell_b^2, \tag{A8}
\end{aligned}$$

and

$$\mathcal{S}^{(2)} = n_h \left(-\frac{2}{3}\ell_b^2 + \frac{10}{9}\ell_b - \frac{14}{27} \right), \tag{A9}$$

where $\ell_b = -\log(m_b/\mu_R)$. To match the implementation of the amplitudes in a 4FS calculation, we then convert the expansion in $\alpha_s^{n_f}$ of $\bar{\mathcal{F}}$, $\bar{\mathcal{S}}$, and the squared finite remainders into an expansion in the coupling constant $\alpha_s^{n_l}$ of the effective theory with n_h decoupled quarks [80] through a finite renormalization shift

$$\alpha_s^{n_f} = \alpha_s^{n_l} \left\{ 1 + \left(\frac{\alpha_s^{n_l}}{2\pi} \right) \frac{2}{3}\ell_b n_h + \left(\frac{\alpha_s^{n_l}}{2\pi} \right)^2 \left[\frac{4}{9}\ell_b^2 n_h^2 + \ell_b n_h \left(\frac{5}{3}C_A + C_F \right) + n_h \left(-\frac{4}{9}C_A + \frac{15}{8}C_F \right) \right] \right\}. \tag{A10}$$

We note that in Ref. [81] $\mathbf{Z}^{-1}$ is defined in the effective theory with n_h decoupled quarks. To obtain the expansions in $\alpha_s^{n_f}$ in Eqs. (A3)–(A9), we expand $\mathbf{Z}^{-1}$ in $\alpha_s^{n_f}$ by applying the inverse of the decoupling relation (A10) (Sec. 4.2 of [81]).

Finally, we calculate the two-loop contribution as

$$2\text{Re}\langle \mathcal{R}^{(0)} | \mathcal{R}^{(2)} \rangle = \frac{|\mathcal{R}^{(0)}|^2}{|\mathcal{R}_0^{(0)}|^2} 2\text{Re}\langle \mathcal{R}_0^{(0)} | \mathcal{R}_{m_b \ll \mu_h}^{(2)} \rangle + \mathcal{O}\left(\frac{m_b}{\mu_h}\right), \tag{A11}$$

$$2\text{Re}\langle \mathcal{R}_0^{(0)} | \mathcal{R}_{m_b \ll \mu_h}^{(2)} \rangle = 2\bar{\mathcal{F}}^{(2)} |\mathcal{R}_0^{(0)}|^2 + \bar{\mathcal{F}}^{(1)} 2\text{Re}\langle \mathcal{R}_0^{(0)} | \mathcal{R}_0^{(1)} \rangle + \mathcal{S}^{(2)} 2\text{Re}\langle \mathcal{R}_0^{(0)} | \mathbf{C}_d | \mathcal{R}_0^{(0)} \rangle + 2\text{Re}\langle \mathcal{R}_0^{(0)} | \mathcal{R}_0^{(2)} \rangle. \tag{A12}$$

Here $X^{(i)}$ with $X = \{\mathcal{R}, \bar{\mathcal{F}}, \mathcal{S}\}$ are now the coefficients in the expansion in $\alpha_s^{n_l}$, derived from their expressions expanded in $\alpha_s^{n_f}$ above and the expansion of the squared finite remainders in $\alpha_s^{n_f}$ using the decoupling relation in Eq. (A10). The logarithmic contributions in m_b are fully contained within the first three terms of Eq. (A12), while the two-loop diagrams are contained in the massless finite remainder at second order $\text{Re}\langle \mathcal{R}_0^{(0)} | \mathcal{R}_0^{(2)} \rangle$, which

we obtain from the analytic results of Ref. [27]. Since the results of Ref. [27] are obtained in the ‘‘Catani scheme’’ [82], we perform a finite renormalization shift (see, e.g., Ref. [83]) to convert them into the scheme employed here. The coefficients $\kappa_{c\bar{c},i}$ of $\log(m_b/\mu_R)$ powers in Eq. (4) are then obtained from the first three terms on the right-hand side of Eq. (A12) using the results of Eqs. (A3)–(A10).

APPENDIX B: MOMENTUM MAPPINGS

In our 4FS calculation, the phase-space integration is performed assuming massive bottom quarks with $m_b \neq 0$. However, the massless finite remainder $\mathcal{R}_0$ entering Eq. (A11) must be evaluated on on-shell phase-space points P_0 with $m_b = 0$. We therefore need an explicit mapping of massive phase-space points P , $\eta: P \rightarrow P_0$, such that $\eta(P) = P_0 + \mathcal{O}(m_b/\mu_h)$. In addition, we have to ensure that η does not cause $\mathcal{R}_0$ to be evaluated near its singularities. Since the quark- and gluon-initiated channels have distinct leading-order momentum flows (see Fig. 1), it is useful to employ dedicated mappings $\eta_{q\bar{q}}, \eta_{gg}$ for each of the channels.

Let us first define our notation of the momenta by introducing the process as

$$p(p_1)p(p_2) \rightarrow b(p_b)\bar{b}(p_{\bar{b}})\ell^+(p_{\ell^+})\ell^-(p_{\ell^-}). \quad (\text{B1})$$

For $\eta_{q\bar{q}}$ we perform the simultaneous light-cone decomposition [84] of the massive bottom and antibottom

momenta p_b and $p_{\bar{b}}$, respectively, and determine the massless momenta $\hat{p}_b$ and $\hat{p}_{\bar{b}}$ as

$$\begin{aligned} \hat{p}_b &= \alpha^+ p_b - \alpha^- p_{\bar{b}}, & \alpha^\pm &= \frac{1}{2} \left(1 \pm \left(1 - 4 \frac{m_b^2}{m_{b\bar{b}}} \right)^{-\frac{1}{2}} \right), \\ \hat{p}_{\bar{b}} &= \alpha^+ p_{\bar{b}} - \alpha^- p_b, \end{aligned} \quad (\text{B2})$$

which preserves the total momentum $\hat{p}_{b\bar{b}} \equiv p_{b\bar{b}}$ of the $b\bar{b}$ system and prevents a collinear $g \rightarrow b\bar{b}$ splitting in the quark channel. The mapping $\eta_{q\bar{q}}$ is minimal in the sense that only the bottom-quark momenta are modified.

An undesirable side effect of the mapping $\eta_{q\bar{q}}$ (when applied in the gluon channel) is that $\hat{p}_b$ or $\hat{p}_{\bar{b}}$ can become collinear to the initial-state momenta p_1 or p_2 when the $b\bar{b}$ pair is produced at the threshold. In the gluon channel, this introduces a collinear singularity, and we therefore construct η_{gg} such that it avoids these configurations. First, we set the massless momenta to

$$\hat{p}_x = p_x + \left(\sqrt{1 - \frac{m_b^2 n_x^2}{(p_x \cdot n_x)^2}} - 1 \right) \frac{(p_x \cdot n_x)}{n_x^2} n_x \quad \text{with } x \in \{b, \bar{b}\}, \quad (\text{B3})$$

$$n_x = p_x - p_1 \frac{(p_2 \cdot p_x)}{(p_1 \cdot p_2)} - p_2 \frac{(p_1 \cdot p_x)}{(p_1 \cdot p_2)}, \quad (\text{B4})$$

where n_x are transverse to both p_1 and p_2 . Then, to restore momentum conservation, we consider two options: Either we redistribute $\Delta p_{b\bar{b}} = p_b + p_{\bar{b}} - \hat{p}_b - \hat{p}_{\bar{b}}$ into $\hat{p}_1$ and $\hat{p}_2$, such that $\hat{p}_{12} = \hat{p}_1 + \hat{p}_2 = p_1 + p_2 - \Delta p_{b\bar{b}}$, by performing a Lorentz boost on p_1 and p_2 in the direction $-\hat{p}_{12}$ followed by rescaling with $\sqrt{\hat{p}_{12}^2/p_{12}^2}$; or, we redistribute $\Delta p_{b\bar{b}}$ into the lepton momenta $\hat{p}_{\ell^+}$ and $\hat{p}_{\ell^-}$ instead. We have verified that, in both cases, η_{gg} avoids the collinear singularities in the massless amplitudes, but we choose the first option as our default choice, since it leaves the Z momentum untouched. Comparing the two choices, we estimated the uncertainty introduced by the mapping in the gluon channel to be at the subpercent level and roughly of the order of the numerical error of our calculation.

APPENDIX C: FIDUCIAL PHASE-SPACE DEFINITION

In this appendix, we specify the set of fiducial cuts defined in the CMS analysis of Ref. [15] and used in this paper for the comparison to data. The final state under consideration contains a Z boson, decaying either to electrons or muons, and at least one (or two) b jets.

The Z -boson candidate is reconstructed from two same-flavor leptons with opposite charge, with their invariant mass $m_{\ell^+\ell^-}$ in the window $71 \leq m_{\ell^+\ell^-} \leq 111$ GeV. The leptons are required to satisfy the constraint on their transverse momentum of $p_T^\ell > 25$ GeV and a requirement on their pseudorapidity of $|\eta^\ell| < 2.4$. Events with more than two leptons satisfying these cuts are vetoed. In addition, the leading lepton must satisfy the constraint $p_T^{\ell_1} > 35$ GeV. The leptons are “dressed” by adding the momenta of all photons within a radius of $\Delta R^{\gamma, \ell} \leq 0.1$.

Jets are defined by clustering all light partons plus the bottom quark using the anti- k_T algorithm with a radius of $R = 0.4$. They are classified as b jets if they contain at least one bottom-flavored hadron and if they fulfill the transverse-momentum and pseudorapidity thresholds of $p_T^{b\text{-jet}} > 30$ GeV and $|\eta^{b\text{-jet}}| < 2.4$, respectively. In the $Z + \geq 1$ b -jet and $Z + \geq 2$ b -jet fiducial regions, a reconstructed Z boson and at least one or two b jets are required, respectively. The overlap between the leptons (from the Z -boson decay) and the b jets is removed by requiring a minimum distance of $\Delta R^{\ell, b\text{-jet}} > 0.4$ between them.

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