EAST EUROPEAN JOURNAL OF PHYSICS
East Eur. J. Phys. **1**. 40-45 (2019) DOI:10.26565/2312-4334-2019-1-03

PACS: 12.38.Bx, 14.65.Dw, 14.65.Fy, 13.85.-t

PRODUCTION OF $c\bar{c}$ – AND $b\bar{b}$ – QUARK PAIRS IN pp COLLISIONS AT ENERGIES OF EXPERIMENTS AT THE LARGE HADRON COLLIDER

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Received December 29, 2018; revised February 4, 2019; accepted February 14, 2019

Production of charm and beauty quark–antiquark pairs in proton–proton collisions is simulated with the codes generated in the framework of MadGraph5_aMC@NLO. The tree–level partonic processes are taken into account in first three orders of the perturbative quantum chromodynamics. The considered hard processes have two, three, and four partons in the final states. These final states contain one or two heavy quark–antiquark pairs. The calculations are performed with parton distribution functions (PDF) obtained with neural network methods by NNPDF collaboration. Influence of the multiple partonic interactions (MPI), initial– and final–state showers on the cross sections (CSs) is studied consistently taking advantage of Pythia 8 event generator. The CSs are computed in central and forward rapidity regions under conditions of the ALICE and LHCb experiments at the Large Hadron Collider at CERN. The studied transverse momentum interval of the heavy quarks spreads up to 30 GeV/c. The CSs calculated at the leading order (LO) with Pythia 8, in the tree approximation with MadGraph5, and within Fixed Order plus Next–to–Leading Logarithms (FONLL) approach agree with each other within bands of the uncertainties inherent to underlying theory and methods. Inclusion of next–to–leading order (NLO) and N^{2}LO partonic processes into calculations in addition to LO ones results in growth of the CSs. This increase reduces to some extent discrepancies with the CSs measured by ALICE and LHCb. Variations of the CSs due to renormalization– and factorization–scale dependence are much larger than the increase of the CSs in NLO and N^{2}LO, than the uncertainties springing in the NNPDF model, and then the accuracy achieved in the ALICE and LHCb cross section measurements. Effects of the MPI, the space– and time–like partonic showers on the heavy quark CSs are found to be not very essential.
KEYWORDS: charm and bottom quark, LHC, ALICE, LHCb, MadGraph5_aMC@NLO, Pythia 8

НАРОДЖЕННЯ $c\bar{c}$ – ТА $b\bar{b}$ – КВАРКОВИХ ПАР В pp ЗІТКНЕННЯХ ПРИ ЕНЕРГІЯХ ЕКСПЕРИМЕНТІВ НА ВЕЛИКОМУ АДРОННОМУ КОЛАЙДЕРІ

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Народження зачарованих і боттом кварк–антикваркових пар в протон–протонних зіткненнях моделюється за допомогою комп'ютерних програм, що було сгенеровано за допомогою MadGraph5_aMC@NLO. Деревинні партонні процеси враховуються в перших трьох порядках теорії збурень у квантовій хромодинаміці. Розглянуті жорсткі процеси мають два, три та чотири партони в кінцевих станах. Ці кінцеві стани містять одну або дві пари важких кварк-антикварків. Розрахунки виконуються з функціями розподілу партонів, отриманих колабораціэю NNPDF з використанням методів нейронних мереж. Вплив багаторазових партонних взаємодій, злив в початковому та кінцевому станах на інтегральні перерізи (ІП) вивчається узгоджено з використанням ґенератора подій Pythia 8. ІП обчислюються в центральній області бистрот та під малими кутами емісії важких кварків за умовами експериментів ALICE та LHCb на Великому адронному колайдері ЦЕРН. Реакції досліджено при поперечних імпульсах важких кварків до 30 ГэВ /с. ІП, що було розраховано в лідируючому порядку (ЛП) з Pythia 8, в деревинному наближенні з MadGraph5, а також на основі FONLL–підходу, узгоджуються між собою в межах смуг невизначеностей властивих теорії та методам, що використовуються. Включення у розрахунки партонних процесів в наступному за лідируючим порядку (НЛП) і Н^{2}ЛП на додаток до ЛП приводить до зростання ІП. Це збільшення зменшує неузгодженість з перерізами, що було отримано ALICE та LHCb. Варіації ІП, пов'язані зі шкалами перенормування та факторизації, значно перевищують отримане збільшення ІП в НЛП та Н^{2}ЛП, невизначеності моделі NNPDF, і точність вимірів перерізів, які було виконано ALICE та LHCb. Багаторазові партонні взаємодії, просторово- та часо-подібні партонні зливи не змінюють суттєво ІП.
КЛЮЧОВІ СЛОВА: зачаровані і боттом кварки, LHC, ALICE, LHCb, MadGraph5_aMC@NLO, Pythia 8

РОЖДЕНИЕ $c\bar{c}$ – И $b\bar{b}$ – КВАРКОВИХ ПАР В pp СТОЛКНОВЕНИЯХ ПРИ ЕНЕРГИЯХ ЕКСПЕРИМЕНТОВ НА БОЛЬШОМ АДРОННОМ КОЛЛАЙДЕРЕ

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Рождение очарованных и боттом кварк-антикварковых пар в протон–протонных столкновениях моделируется с помощью компьютерных программ, которые были получены с помощью MadGraph5_aMC@NLO. Древесные партонные процессы

учитываются в первых трех порядках теории возмущений квантовой хромодинамики. Рассматриваются жесткие процессы с двумя, тремя и четырьмя партонами в конечных состояниях. Эти конечные состояния содержат одну или две пары тяжелых кварк-антикварков. Расчеты выполняются с функциями распределения партонов, полученными коллаборацией NNPDF с использованием методов нейронных сетей. Влияние многократных партонных взаимодействий, ливней в начальном и конечном состояниях на интегральные сечения (ИС) изучается согласованно с генератором событий Pythia 8. ИС вычисляются в центральной области быстрот и под малыми углами эмиссии тяжелых кварков в условиях экспериментов ALICE и LHCb на Большом адронном коллайдере ЦЕРН. Реакции исследуются при поперечных импульсах тяжелых кварков до 30 ГэВ/с. ИС, рассчитанные в лидирующем порядке (ЛП) с Pythia 8, в древесном приближении с MadGraph5, а также на основе FONLL-подхода, согласуются между собой в пределах полос неопределенностей, присущих используемым теории и методам. Включение в расчеты партонных процессов в следующем за лидирующим порядке (НЛП) и Н^{2}ЛП в дополнение к ЛП приводит к росту ИС. Это увеличение уменьшает рассогласование с сечениями, которые были получены ALICE и LHCb. Вариации ИС, связанные со шкалами перенормировки и факторизации, значительно превышают полученное увеличение ИС в НЛП и Н^{2}ЛП, неопределенности модели NNPDF, а также точность измерений сечений, которые были выполнены ALICE и LHCb. Изменения ИС при учёте многократных партонных взаимодействий, пространственно и времени–подобных партонных ливней не являются существенными.
КЛЮЧЕВЫЕ СЛОВА: очарованные и боттом кварки, LHC, ALICE, LHCb, MadGraph5_aMC@NLO, Pythia 8

Open charm and beauty production is a subject of intensive experimental and theoretical researches. The heavy quarks, D– and B–mesons, baryons that contain *c*– or *b*–quarks are detected in the LHC experiments ALICE, ATLAS, CMS, and LHCb. The integral and differential CSs of the processes are obtained making available excellent testing grounds for calculations within perturbative quantum chromodynamics (pQCD) and for QCD–motivated phenomenological models that incorporate non–perturbative effects. Provided that the reaction mechanisms are under strict control, heavy flavor production can be also a tool to investigate gluon distribution properties in protons and nuclei. Various frameworks and event generators (EGs), e.g. FONLL approach [1,2], MadGraph5_aMC @ NLO [3], Pythia 8 [4], POWHEG-BOX [5], HERWIG [6], Sherpa [7], along with the PDF model, e.g. NNPDF [8], are employed for interpretation of the data.

An objective of this paper is to simulate processes of heavy quark production at the LHC energies under conditions of ALICE [9] and LHCb [10,11] experiments. ALICE measurements in central rapidity region $|y| \leq 0.5$ compliment the LHCb studies at pseudorapidities $2 \leq \eta \leq 5$. Area of relatively small transverse momenta $p_T \lesssim 20 \ldots 30$ GeV/c can be explored by both detectors. We aim to carry out calculations of the cross section for charmed and bottom quark production at LO, NLO and at N^{2}LO within the tree approximation of pQCD and to demonstrate how corrections beyond LO affect the CSs. MadGraph5_aMC @ NLO and Pythia 8 are to be used with this end. Results of calculations are to be compared with the experimental data and theoretical uncertainties are to be discussed.

SIMULATION OF HEAVY QUARK PRODUCTION BEYOND LEADING ORDER OF PERTURBATIVE QUANTUM CHROMODYNAMICS

Heavy quark anti–quark pairs are created in hard partonic processes, e.g. $g + g \to Q + \bar{Q}$, where Q is charmed or bottom quark. Codes for modeling these processes in proton–proton scattering are generated with MadGraph5_aMC @ NLO [3] in the tree approximation. Calculations are performed for groups of processes

$$p + p \to Q + \bar{Q}, \tag{1}$$

$$p + p \to Q + \bar{Q},\ \ Q + \bar{Q} + jet, \tag{2}$$

$$p + p \to Q + \bar{Q},\ \ Q + \bar{Q} + jet,\ \ Q + \bar{Q} + 2jet,\ \ 2(Q + \bar{Q}), \tag{3}$$

that have from two up to four partons in the final sates. In (1) … (3) *p* and *jet* denote gluon or one of the quarks u, d, s for *Q=c* and u, d, s, c for *Q=b*. Particles *p* and *jet* can be respective anti–quarks. In model employed in the simulations charmed and bottom quarks in the final states are massive. In protons and in *jets* quarks u, d, s, c have zero masses. LO Born, NLO, and N^{2}LO gluon scattering that results in $b\bar{b}$ –pair creation at the tree level is illustrated in Fig. 1. Processes initiated by two gluons together with quark–gluon scattering determine sensitivity of the observables to gluon distribution in colliding hadrons.

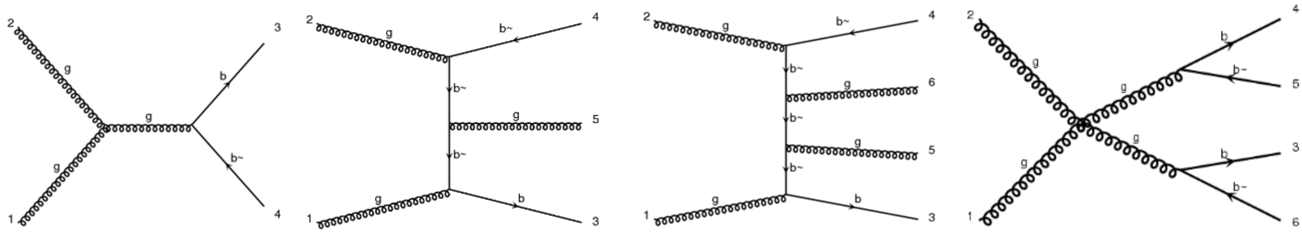

Fig. 1. Gluon interaction that results in final states with two, three, and four particles.
The diagrams are generated by MadGraph

Partonic events obtained with the MadGraph codes are showered then with Pythia 8 [4] and MPI are simulated also with this EG. NNPDF parton distribution functions [8] are used in the computations.

CROSS SECTIONS OF $c\bar{c}-$ AND $b\bar{b}-$ PRODUCTION

Integral cross sections (CS) are calculated with MadGraph5_aMC @ NLO [3] in junction with Pythia 8 [4] at LO, NLO, and N^{2}LO at tree level and with Pythia 8 at LO. Computed CSs are compared with results obtained within FONLL approach [1,2].

As seen from Fig. 2, where CSs integrated over all rapidity range are shown, inclusion of processes with three and four partons in the final states in addition to ones with single $Q\bar{Q}$–pair does not affect the CSs values essentially in comparison with the uncertainties of the CSs that originate from variation of the renormalization and factorization scales. In calculation with MadGraph and Pythia these uncertainties are determined for scale factors from ½ up to 2 that change independently for renormalization and factorization scales. CSs obtained with MadGraph and Pythia, Pythia, and FONLL differ insignificantly.

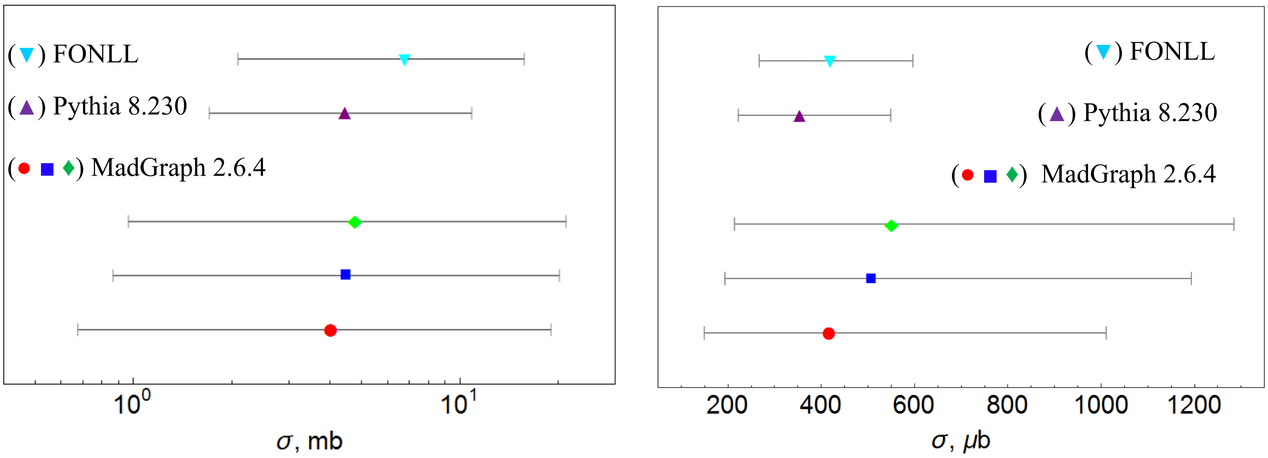

Fig. 2. The CSs of charmed (left) and bottom (right) quark anti–quark pair production in pp collisions at s$^{1/2}$ = 13 TeV. CSs calculated with MadGraph for groups of partonic processes (1), (2), and (3) are shown by ●, ■, and ♦, respectively

In simulations with MadGraph we chose minimal value of jet transverse momenta $p_{T\,jet\,min}$ = 10 GeV/c that is set to be equal to the minimal distance in the momentum space between the partons in accepted events. Solid curves in Fig. 3 demonstrate that the integral CS changes very slowly when $p_{T\,jet\,min}$ exceeds value ~10 GeV/c. Further decrease of the CS from momenta $p_{T\,jet\,min}$ = 20 up to 60 GeV/c is 2.4%. In the present calculations at s$^{1/2}$ = 13 TeV, the integral CSs are obtained for the transverse momenta of the heavy quarks $p_{T\,c\,min}$ and $p_{T\,b\,min}$ = 0. Swift decline of the CS with growth of $p_{T\,c\,min}$ is illustrated by the dashed curve in fig. 3. This decrease of the CS is followed by reduction of the scale uncertainties as shown in Fig. 4. Thus, positive uncertainty falls from 348% at $p_{T\,c\,min}$ = 0 down to 127% at $p_{T\,c\,min}$ = 5 GeV/c and then to 88.6% at $p_{T\,c\,min}$ = 20 GeV/c.

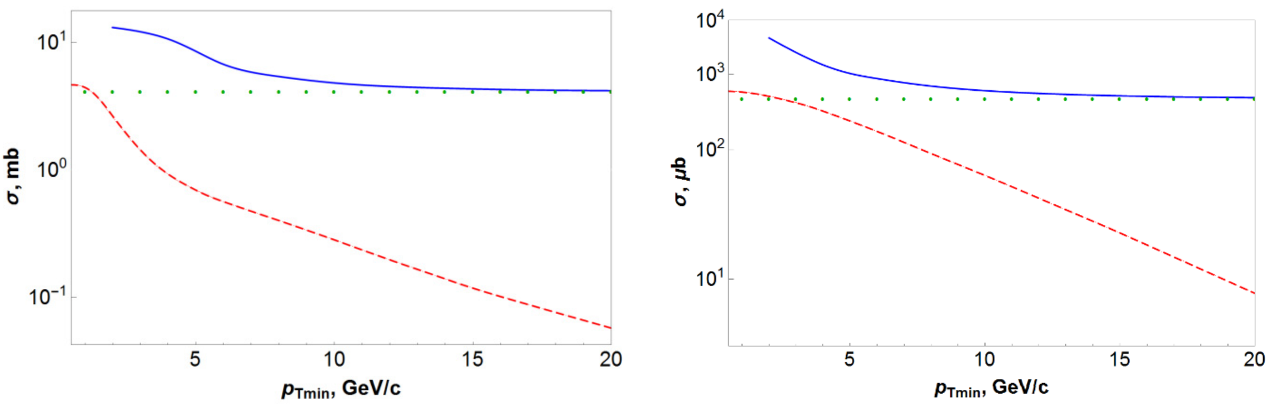

Fig. 3. The integral CSs for production of $c\bar{c}$–quarks (left) and $b\bar{b}$–quarks (right) at s$^{1/2}$ = 13 TeV. The CSs $\sigma(p_{T\ jet\ min},\ p_{T\ Q\ min}=0)$ and $\sigma(p_{T\ jet\ min}=10\ GeV/c,\ p_{T\ Q\ min})$ at N^{2}LO are shown by solid and dashed curves, dots — CSs at LO of pQCD. Heavy quark Q is charmed or bottom one

The CSs of charmed and bottom quark production in central rapidity region |y| < 0.5 are compared in Fig. 5 with the ALICE data. The experimental values of the heavy quark differential CS at $y=0$, shown in Fig. 5, have been extracted in [9] from the ALICE data on dielectron production. Within approach [9] simulation with EGs is employed. Results [9] obtained with PYTHIA and POWHEG [5] are indicated by up ▲ and down ▼ triangles.

The CSs of heavy quark production in the forward rapidity region are shown in Fig. 6 together with the LHCb data. As can be seen from Fig. 5 and Fig. 6 results of calculations for bottom quarks do not contradict to the results of

ALICE and LHCb measurements. Experimental data for charmed quark CSs lie within the scale variations of the calculations.

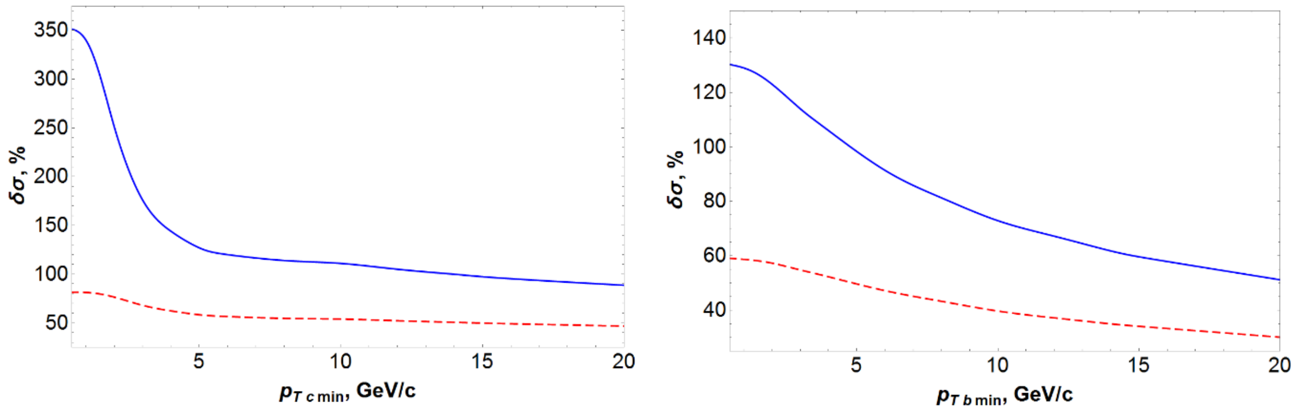

Fig. 4 Scale uncertainties of the $c\bar{c}$–quarks (left) and $b\bar{b}$–quarks (right) production CSs as functions of $p_{T\,Q\,min}$, where Q is for c– and b–quarks. Solid and dashed curves are for positive and negative CS variations

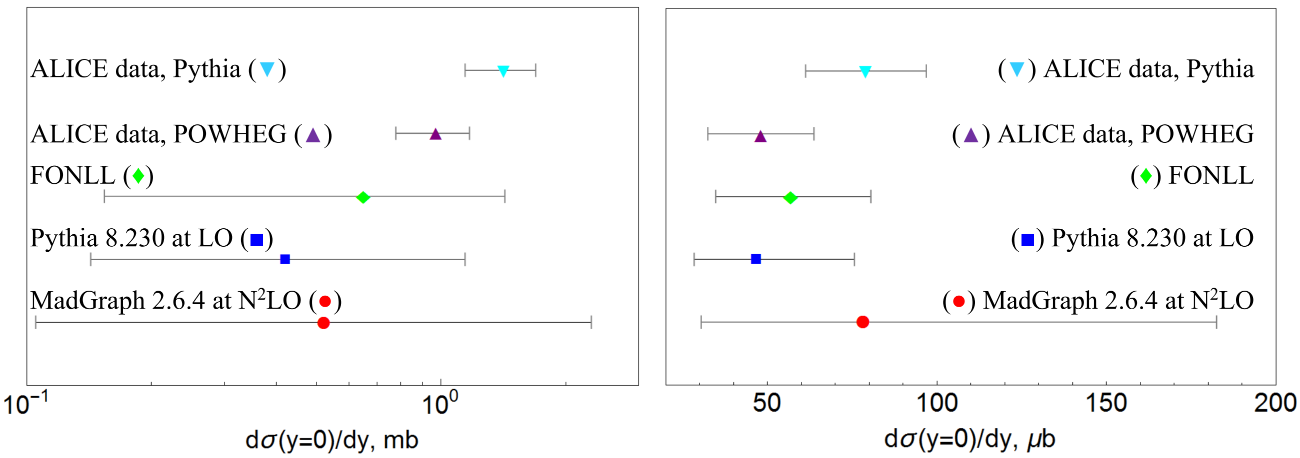

Fig. 5. The differential CSs of $c\bar{c}$ (left) and $b\bar{b}$ (right) production at zero rapidity in pp scattering at $s^{1/2}$ = 13 TeV. The ALICE data ▲ and ▼ are taken from [9]

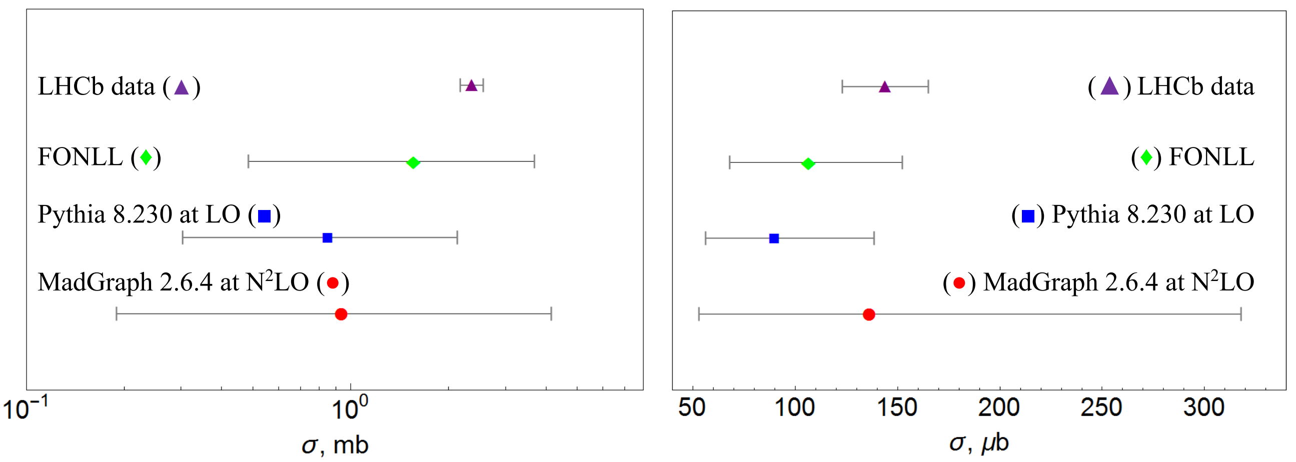

Fig. 6. The integral CSs for charmed (left) and bottom (right) quark anti–quark pair production in the forward rapidity region in pp scattering at $s^{1/2}$ = 13 TeV. The LHCb data ▲ are from [10,11]

The differential CSs of bottom quark production as function of pseudorapidity η that are obtained with MadGraph 5 and Pythia 8 at the tree level at N^{2}LO are compared in Fig. 7 with the LHCb data. Note that being dependent on total energy $s^{1/2}$ and interval of integration over the transverse momenta, the relative size of scale uncertainties for η–distributions in Fig. 7 keeps constant regardless of the values η takes.

As seen from Fig. 7, the experimental CS η–dependences have maxima. At $s^{½}$ = 13 TeV this feature of the CS is more distinct then in the data at 7 TeV. The calculations do not reproduce this behavior of CS $d\sigma/d\eta$. The reasons for this discrepancy may be caused by use of the tree approximation or by choice of some cut-off in the phase space that are not in full correspondence with the measurement procedure and the data analysis.

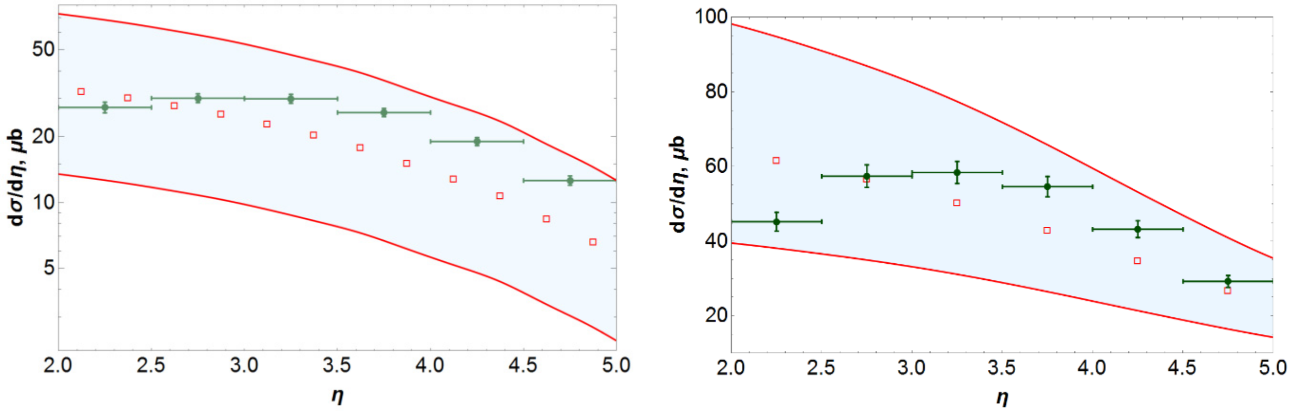

Fig. 7. The differential CSs for $b\bar{b}$–pair production in pp scattering at $s^{1/2}$ = 7 (left) and 13 TeV (right). Calculations with MadGraph 5 and Pythia 8 are shown by squares □, the scale uncertainties — by the band. The LHCb data ● are from [11]

Figs. 5-7, in which the results of simulations are compared with the LHC data, demonstrate that for all measurements the experimental uncertainties are smaller as compared with theoretical ones.

CONCLUSIONS

Charmed and bottom quark production in proton–proton scattering is simulated at $s^{1/2}$ = 7 and 13 TeV. Calculations are performed at the tree level of pQCD with the codes for hard partonic processes, generated by MadGraph5_aMC @ NLO [3]. First three order of QCD perturbation theory are taken into account. Space– and time–like partonic showers, multiparton interactions are included into the modeling with the help of Pythia 8 [4] event generator.

The integral cross sections of *c* and *b* quark anti–quark pair production are calculated both in the central and forward rapidity regions under conditions of ALICE [9] and LHCb [10,11] experiments. The pseudorapidity dependence of the differential cross section for $b\bar{b}$–pair production is also computed in the LHCb kinematic area. NLO and N^{2}LO contributions increase the integral cross sections and results obtained with MadGraph5_aMC@NLO in junction with Pythia 8 at N^{2}LO are in agreement with the ALICE and LHCb data within the band of uncertainties due to renormalization and factorization scale variations. At the same time, the $b\bar{b}$ differential cross sections at 7 and 13 TeV as functions of pseudorapidity differ in form from ones measured by the LHCb.

Calculations show that the influence of NLO and N^{2}LO terms on the integral cross sections reduces with growth of jet minimal transverse momenta and at $p_{T\ \mathrm{jet\ min}} \sim 10$ GeV/c becomes inessential. In the present simulation, the value of $p_{T\,jet\,min}$ equals the minimal distance in phase space between the partons in final states of hard processes. Thus, selection of events with well-separated jets together with elimination of events with soft jets can be used to suppress the contributions springing beyond LO in pQCD, to simplify the relevant reaction mechanisms, and to enhance sensitivity of the observables to the parton distributions functions, in particular to gluon ones.

Changes in the computed cross sections under scale variations turn out to be much larger than experimental uncertainties. Rapid exponential decrease of the cross sections with increase of minimal transverse momenta $p_{T\,Q\,min}$ of the heavy quark, $Q = c$ or b, is followed by reduction of the scale uncertainty size. It appears to be significant in the case of charmed quarks. Region of $p_{T\,c\,min} \gtrsim 5$ GeV/c, where strip width of these uncertainties narrows, proves to be suitable for verification of the pQCD methods and of QCD–based models, employed in the simulations.

No substantial effect of partonic showers and multiparton interactions on the integral cross sections under considered kinematic cut-offs is found. Influence of these mechanisms on differential observables needs further studying.

ACKNOWLEDGMENTS

V.V.K. acknowledges partial support of these researches by the National Academy of Sciences of Ukraine (project no. 0118U006495) and by the Ministry of Education and Science of Ukraine (project no. 0117U004866).

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