Title
Distributions of topological observables in inclusive three- and four-jet events in pp collisions at [Formula: see text][Formula: see text].

Journal
The European physical journal. C, Particles and fields, 75(7)

ISSN
1434-6044

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Publication Date
2015

DOI
10.1140/epjc/s10052-015-3491-9

Eur. Phys. J. C (2015) 75:302
DOI 10.1140/epjc/s10052-015-3491-9

THE EUROPEAN PHYSICAL JOURNAL C

Regular Article - Experimental Physics

Distributions of topological observables in inclusive three- and four-jet events in pp collisions at $\sqrt{s} = 7$ TeV

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Received: 16 February 2015 / Accepted: 2 June 2015 / Published online: 1 July 2015

Abstract This paper presents distributions of topological observables in inclusive three- and four-jet events produced in pp collisions at a centre-of-mass energy of 7 TeV with a data sample collected by the CMS experiment corresponding to a luminosity of 5.1 fb^{-1}. The distributions are corrected for detector effects, and compared with several event generators based on two- and multi-parton matrix elements at leading order. Among the considered calculations, MADGRAPH interfaced with PYTHIA6 displays the overall best agreement with data.

1 Introduction

In proton-proton collisions at the LHC, interactions take place between the partons of the colliding protons. The scattered partons from hard collisions fragment and hadronize into collimated groups of particles called jets. The study of jets with high transverse momentum (p_T) provides a test of the predictions from quantum chromodynamics (QCD) and deviations from these predictions can be used to look for physics beyond the standard model. While parton scattering is an elementary QCD process that can be calculated from first principles, predictions of jet distributions require an accurate hadronization model. In this paper, several hadronization models are examined.

High-p_T parton production is described by perturbative QCD (pQCD) in terms of the scattering cross section convolved with a parton distribution function (PDF) for each parton that parametrizes the momentum distribution of partons within the proton. The hard-scattering cross section itself can be written as an expansion in the strong coupling constant α_s. The leading term in this expansion corresponds to the emission of two partons. The next term includes diagrams where an additional parton is present in the final state as a result of hard-gluon radiation (e.g. gg $\rightarrow$ ggg). Cross sections for such processes diverge when any of the three partons becomes soft or when two of the partons become collinear. Finally, pQCD predicts three classes of four-jet events that correspond to the processes qq/gg $\rightarrow$ qqgg, qq/gg $\rightarrow$ qqqq and qg $\rightarrow$ qggg/qqqg, where q stands for both quarks and anti-quarks. Processes with two or more gluons in the final state receive a contribution from the triple-gluon vertex, a consequence of the non-Abelian structure of QCD.

We are studying distributions of topological variables, which are sensitive to QCD color factors, the spin structure of gluons, and hadronization models. These topological variables were studied widely in the earlier LEP [1,2] and the Tevatron [3,4] experiments and help to validate theoretical models implemented in various Monte Carlo (MC) event generators.

The distributions of multijet variables are sensitive to the treatment of the higher-order processes and approximations involved. Many MC event generators make use of leading order (LO) matrix elements (ME) in the primary 2 $\rightarrow$ 2 process. A good agreement between the measurements and MC predictions can establish the validity of the treatment of higher-order effects, and any large deviation may lead to large systematic uncertainties in searches for new physics.

The multijet observables presented here are based on hadronic events from 7 TeV pp collision data recorded with the CMS detector corresponding to an integrated luminosity of 5.1 fb^{-1}. The kinematic and angular properties of these events are computed from the jet momentum four-vectors. Unfolding techniques are used to correct for the effects of the detector resolution and efficiency. Systematic uncertainties resulting from the limited knowledge of the jet energy scale (JES), jet energy and angular resolution (JER), unfolding, and event selection are estimated, and the unfolded distributions are compared with predictions of several QCD-based MC models.

In this paper, the CMS detector is briefly described in Sect. 2. Sections 3 and 4 summarize the MC models used and the variables studied in this paper. Event selection and measurements are described in Sects. 5 and 6, respectively. The correction of the distributions due to detector effects is

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discussed in Sect. 7. Sections 8 and 9 describe the estimation of systematic uncertainties and the final results. The overall summary is given in Sect. 10.

2 The CMS detector

The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, providing a magnetic field of 3.8 T. Within the field volume are a silicon pixel and strip tracker, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter (HCAL), each composed of a barrel and two endcap sections. Muons are measured in gas-ionization detectors embedded in the steel flux-return yoke outside the solenoid. Extensive forward calorimetry complements the coverage provided by the barrel and endcap detectors. The barrel and endcap calorimeters cover a pseudorapidity region $-3.0 < \eta < 3.0$. Pseudorapidity is defined as $\eta = -\ln\tan[\theta/2]$, where θ is the polar angle. The transition between barrel and endcaps happens at $|\eta| = 1.479$ for the ECAL and $|\eta| = 1.15$ for the HCAL. The first level (L1) of the CMS trigger system, composed of custom hardware processors, uses information from the calorimeters and muon detectors to select the most interesting events in a fixed time interval of less than 4 μs. The high-level trigger (HLT) processor farm further decreases the event rate from around 100 kHz to around 400 Hz before data storage. A more detailed description of the CMS detector, together with a definition of the coordinate system used and the relevant kinematic variables, can be found in Ref. [5].

3 Monte Carlo models

The MC event generators rely on models using modified LO QCD calculations. The elementary hard process between the partons is computed at LO. The parton shower (PS), used to simulate higher-order processes, follows an ordering principle motivated by QCD. Nevertheless, the parton shower models can differ in the ordering of emissions and the event generators can also have different treatments of beam remnants and multiple interactions.

The PYTHIA 6.4.26 [6] event generator uses a PS model to simulate higher-order processes [7–9] after the LO ME from pQCD calculations. The PS model, ordered by the p_T of the emissions, provides a good description of event shapes when the emitted partons are close in phase space. Events are generated with the Z2 tune [10] for the underlying event. This tune is identical to the Z1 tune [11], except that it uses CTEQ6L1 [12] PDFs. The partons are hadronized (process of converting the partons into measured particles) using the Lund string model [13,14].

The PYTHIA 8.153 [15] event generator also uses a PS model with the successive emissions of partons ordered in p_T and the Lund string model for hadronization. The main difference between the two PYTHIA versions is the description of multiparton interactions (MPI). In PYTHIA8, initial state radiation (ISR), final state radiation (FSR), and MPI are interleaved in the p_T ordering, while in PYTHIA6, only ISR and FSR are interleaved. The tune 4C [16] is used with this generator. This tune uses CTEQ6L1 PDFs with parameters using CDF as well as early LHC measurements.

The HERWIG++ 2.4.2 [17] tune 23 [18] program takes the LO ME and simulates a PS using the coherent branching algorithm with angular ordering [19] of the showers. The partons are hadronized in this model using a cluster model [20] and the underlying event is simulated using the eikonal multiple partonic scattering model.

In the case of MADGRAPH 5.1.5.7 [21], multiparton final states are also computed at tree level. The parton shower and nonperturbative parts for MADGRAPH 5.1.5.7 simulation sample is handled by PYTHIA 6.4.26 with Z2 tune. The MLM matching procedure [22] is used to avoid double counting between the ME and the PS. The MADGRAPH samples are created in four bins of the variable H_T, the scalar sum of the parton p_T. The matching between ME and PS has been studied in detail and has been validated using inclusive jet p_T distributions. Several samples are generated using different matching parameters and are used in estimating systematic uncertainty in the theoretical prediction.

These MC programs are the most commonly used models to describe multi-partonic final states and are normally used to describe QCD background in searches within CMS. The events produced from these models are simulated using a CMS detector simulation program based on GEANT4 [23] and reconstructed with the same program used for the data. These MC events are used for the comparison with the measurements as well as to correct the distributions for detector effects.

4 Definition of variables

4.1 Three-jet variables

The topological variables used in this study are defined in the parton or jet centre-of-mass (CM) system. The topological properties of the three-parton final state in the CM system can be described in terms of five variables [3]. Three of the variables reflect partition of the CM energy among the three final-state partons. There are three angles, which define the spatial orientation in the plane containing the three partons, but only two are independent.

It is convenient to introduce the notation $1+2 \rightarrow 3+4+5$ for the three-parton process. Here, numbers 1 and 2 refer to

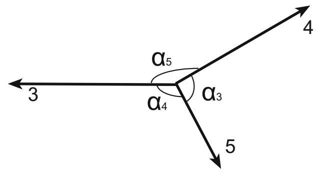

Fig. 1 Illustration of the three-jet variables in the process 1+2→3+4+5. The scaled energies are related to the angles (α_i) among the jets for massless parton

incoming partons while the numbers 3, 4, and 5 label the outgoing partons in a descending order in energies in the parton CM frame, i.e. $E_3 > E_4 > E_5$ (Fig. 1). The final-state parton energy is an obvious choice for the topological variable for the three-parton final state. For simplicity, E_i ($i = 3, 4, 5$) is often replaced by the scaled variable x_i ($i = 3, 4, 5$), which is defined by $x_i = 2E_i/\sqrt{\hat{s}_{345}}$, where $\sqrt{\hat{s}_{345}}$ is the CM energy of the hard-scattering process. It is also referred to as the mass of the three-parton system, and by definition,

$$x_3 + x_4 + x_5 = 2. \quad (1)$$

The internal structure of the three-parton final state is determined by any two scaled parton energies. The third one is calculated using Eq. 1. It needs two angular variables which fix the event orientation. In total, five independent kinematic variables are needed to describe the topological properties of the three-parton final state. In this analysis, however, the study is restricted to three variables: $\sqrt{\hat{s}_{345}}$, x_3, and x_4, while the angular variables are not included.

4.2 Four-jet variables

To define a four-parton final state in its CM frame, eight independent parameters are needed. Two of these define the overall event orientation, while the other six fix the internal structure of the four-parton system. In contrast to the three-parton final state, there is no simple relationship between the scaled parton energies and the opening angles between partons. Consequently, the choice of topological variables is less obvious in this case. Variables are defined here in a way similar to those investigated for the three-parton final state. The four partons are ordered in descending energy in the parton CM frame and labeled from 3 to 6. The variables include the scaled energies and the polar angles of the four partons with respect to the beams.

In addition to the four-parton CM energy or the mass of the four-parton system ($\sqrt{\hat{s}_{3456}}$), two angular distributions characterizing the orientation of event planes are investigated. One of these is the Bengtsson–Zerwas angle (χ_{BZ}) [24] defined as the angle between the plane containing the two leading jets and the plane containing the two nonleading jets:

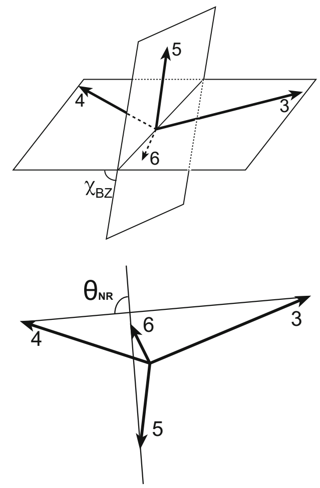

Fig. 2 Illustration of the Bengtsson–Zerwas angle (χ_{BZ}) and the Nachtmann–Reiter angle (θ_{NR}) definitions for the four-jet events. The *top figure* shows the Bengtsson–Zerwas angle, which is the angle between the plane containing the two leading jets and the plane containing the two nonleading jets. The *bottom figure* shows the Nachtmann–Reiter angle, which is the angle between the momentum vector differences of the two leading jets and the two nonleading jets

$$\cos\chi_{BZ} = \frac{(\mathbf{p}_3 \times \mathbf{p}_4)\cdot(\mathbf{p}_5 \times \mathbf{p}_6)}{|\mathbf{p}_3 \times \mathbf{p}_4||\mathbf{p}_5 \times \mathbf{p}_6|}. \quad (2)$$

The second variable is the cosine of the Nachtmann–Reiter angle ($\cos\theta_{NR}$) [25] defined as the angle between the momentum vector differences of the two leading jets and the two nonleading jets:

$$\cos\theta_{NR} = \frac{(\mathbf{p}_3 - \mathbf{p}_4)\cdot(\mathbf{p}_5 - \mathbf{p}_6)}{|\mathbf{p}_3 - \mathbf{p}_4||\mathbf{p}_5 - \mathbf{p}_6|}. \quad (3)$$

Figure 2 illustrates the definitions of χ_{BZ} and θ_{NR} variables. Historically, χ_{BZ} and θ_{NR} were proposed for e^+e^- collisions to study gluon self-coupling. Their interpretation in pp collisions is more complicated, but the variables can be used as a tool for studying the internal structure of the four-jet events.

5 Data samples and event selection

Jets are reconstructed from particle-flow (PF) objects [26,27] using the anti-k_T clustering algorithm [28] with the distance parameter $R = 0.5$, as calculated with FASTJET 2.0 [29]. The PF algorithm utilizes the best energy measurements of each particle candidate from the most suitable combination of the detector components. A cluster is formed from all the particle-flow candidates that satisfy the chosen distance parameter. The four-momentum of the jet is then defined as the sum of four-momenta of the corresponding particle-flow candidates, which results in jets with nonzero mass.

Table 1 Prescales, integrated luminosity and offline p_T threshold of the leading jet for different trigger paths. The terminology for Level 1 (L1) triggers as well as HLT includes the jet p_T threshold (in GeV) applicable to the trigger

Period	HLT L1	HLT60 SingleJet36	HLT110 SingleJet68	HLT190 SingleJet92	HLT240 SingleJet92	HLT370 SingleJet92/SingleJet128
2011A	L1 prescale	1–300	1–10	1	1	1
	HLT prescale	15–180	1–5000	1–60	1–24	1
	$\int \mathcal{L}$ (pb^{-1})	0.29	6.16	114.7	392.2	2328
2011B	L1 prescale	50–400	1–20	1–10	1	1
	HLT prescale	80–84	80–1000	10–100	4–30	1
	$\int \mathcal{L}$ (pb^{-1})	0.12	1.12	40.2	136.0	2767
Overall	$\int \mathcal{L}$ (pb^{-1})	0.41	7.29	154.8	528.2	5096
	p_T threshold	110 GeV	190 GeV	300 GeV	360 GeV	500 GeV

Table 2 Threshold of the leading jet p_T for different HLT paths. This paper shows results from two representative trigger paths HLT110 and HLT370

HLT	HLT60	HLT110	HLT190	HLT240	HLT370
Leading jet p_T (GeV)	110–190	190–300	300–360	360–500	>500

The JES correction applied to jets used in this analysis is based on high-p_T jet events generated by PYTHIA6 and then simulated using GEANT4, and in situ measurements with dijet and photon + jet events [30]. An average of ten minimum bias interactions occur in each pp bunch crossing (pileup), and this requires an additional correction to remove the extra energy deposited by these pileup events. The size of the correction depends on the p_T and η of the jet. The correction appears as a multiplicative factor to the jet energy, and is typically less than 1.2 and approximately uniform in η.

Events passing single-jet HLT requirements are used in this analysis. These triggers require jets reconstructed from calorimetric information with the anti-k_T clustering algorithm and with energy corrections applied. Jets are ordered in decreasing jet p_T, and the leading jet p_T is required to be above a certain threshold. As offline jets are reconstructed with the PF algorithm, this may result in a trigger not being fully efficient near the threshold. Trigger efficiencies are studied as a function of the leading jet p_T for all trigger thresholds. Values of the leading jet p_T, where the trigger efficiency is determined to be larger than 99 %, are listed in Table 1. It also summarizes the prescale factors and the effective integrated luminosities collected using the different HLT thresholds.

Jets are selected with restrictive criteria on the neutral energy fractions (both electromagnetic and hadronic components), and all the jets are required to have $p_T > 50$ GeV and absolute rapidity, ($y = (1/2)\ln[(E + p_z)/(E - p_z)]$), $|y| \leq 2.5$. The jet with the highest p_T is required to be above a threshold as given by the requirement from the trigger turn-on curve. To avoid overlap of events from two different HLT paths, the p_T of the leading jet is also required to be less than an upper value. The overall criteria are summarized in Table 2. Though data from all the five trigger paths are studied, figures from two representative trigger paths (the highest p_T threshold and a lower one with good statistical accuracy) are presented in this paper.

Events are selected with at least three jets passing the selection criteria as stated above. Additional selection requirements are also applied to reduce backgrounds due to beam halo, cosmic rays and detector noise. The event must have at least one good reconstructed vertex [31]. Missing transverse energy, E_T^{miss}, is required to be less than $0.3 \sum E_T$, where the summation is over all PF jets. The quantities E_T^{miss} and $\sum E_T$ are obtained from negative vector sum and scalar sum of the transverse momenta of the jets, respectively. A number of event filters [32] accept only those events that have negligible noise in the detector. The jets are ordered in decreasing p_T, and an event with at least three (four) jets satisfying the jet selection criteria is classified as a three-jet (four-jet) event.

6 Measurements

The 4-momenta of all the jets in the three- or four-jet event category are transformed into the CM frame of the three- or four-jet system. The jets are then ordered in decreasing energy. The three- and four-jet variables as described in Sect. 4 are then calculated from the kinematic and angular information of the jets. Since detector resolution varies over the potential kinematic ranges, variable bin widths are adopted for the jet masses and the scaled jet energies, while for angular variables constant bin widths are used.

6.1 Detector-level distributions

The measured distributions of the three- and four-jet variables are compared with predictions from two MC generators (PYTHIA6 and MADGRAPH + PYTHIA6), simulated using the identical detector condition as that in the data. The identical pileup condition is obtained by reweighting the MC simulation to match the spectrum of pileup interactions observed in the data. The size of the reweighting correction is typically less than 1 %. The agreement between the data and the MC predictions is reasonable, so these MC generators are used to correct the measured distributions.

Figures 3 and 4 show the normalized three- and four-jet mass distributions. The data are compared with two different MC programs: PYTHIA6 and MADGRAPH + PYTHIA6, each with two different HLTs with p_{T} thresholds above 110 and 370 GeV. As can be seen from the figures, there is agreement within a few percent between the data and the predictions of these two simulations. The difference between the predictions and the data varies typically from 4 to 10 %. However, there is a systematic deviation observed at high masses where the simulations are higher than the data.

7 Corrections for detector effects

Multijet variables obtained from MC samples may differ from data because of the detector resolution and acceptance. Before comparisons with other experiments or theoretical predictions can be made, detector effects are unfolded into distributions at the final-state particle level. The basic component of the unfolding is the response function, where experimental observables are expressed as a function of theoretical observables. For simplicity, observables are taken in discrete sets, and the response function is replaced by a response matrix. The observed distribution is then unfolded with the inverse of response matrix to obtain a distribution corrected for detector effects. Matrix inversion has potential complications, because it cannot handle large statistical fluctuations and the matrix itself could be singular. Instead, we use the RooUnfold package [33] with the D'Agostini iterative method [34] as the default algorithm and the singular value decomposition method [35] for cross-checks.

The default response matrix is obtained using the PYTHIA6 event generator. Statistical uncertainties are estimated from the square root of the covariance matrix obtained from a variation of the results generated by simulated experiments.

The corrections for detector resolution and acceptance change the shape of the three-jet mass distributions by approximately 10 %, less than 5 % for the scaled energy of nonleading jets, and up to 20 % for the scaled energy of the leading jet. For four-jet variables, corrections applied are of the order of 20 % for the four-jet mass, 10 % for χ_{BZ}, and less than 5 % for $\cos\theta_{\mathrm{NR}}$.

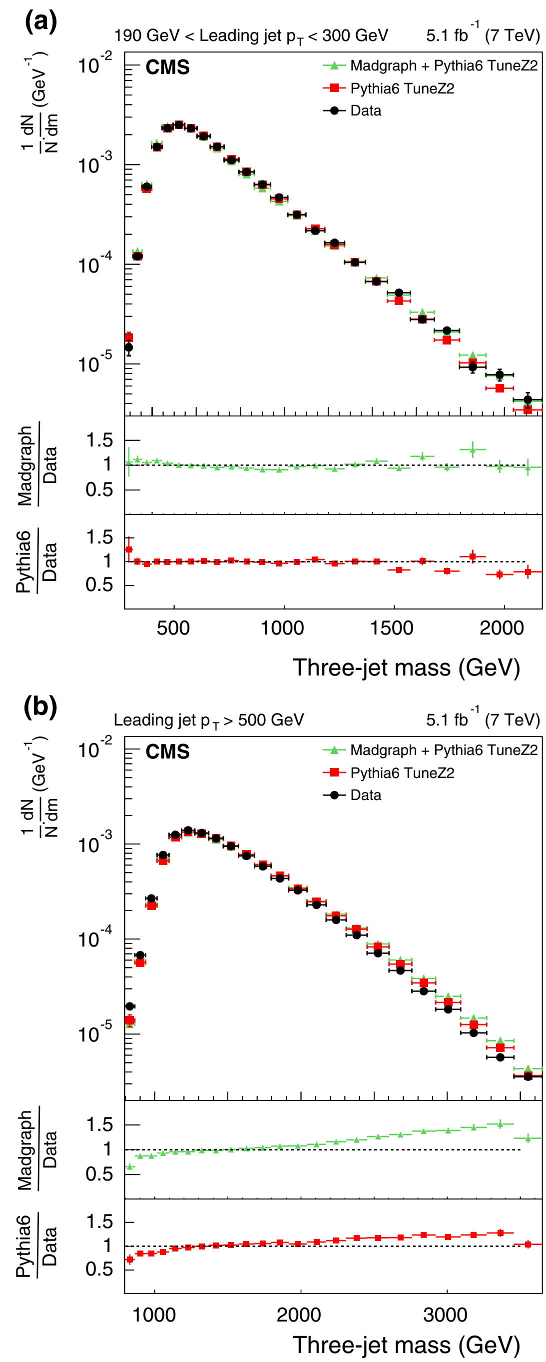

Fig. 3 The *upper panels* display the normalized distributions of the reconstructed three-jet mass for events where the most forward jet has $|y| < 2.5$. *Figures* differ by p_{T} ranges of the leading jet: 190–300 GeV (**a**), and above 500 GeV (**b**) for data (before correction due to detector effects) and predictions from MC generators. The *bottom panel of each plot* shows the ratio of MC predictions to the data. The data are shown with only statistical uncertainty

8 Systematic uncertainties

The leading sources of systematic uncertainty are due to the JES, the JER, and the model dependence of corrections to

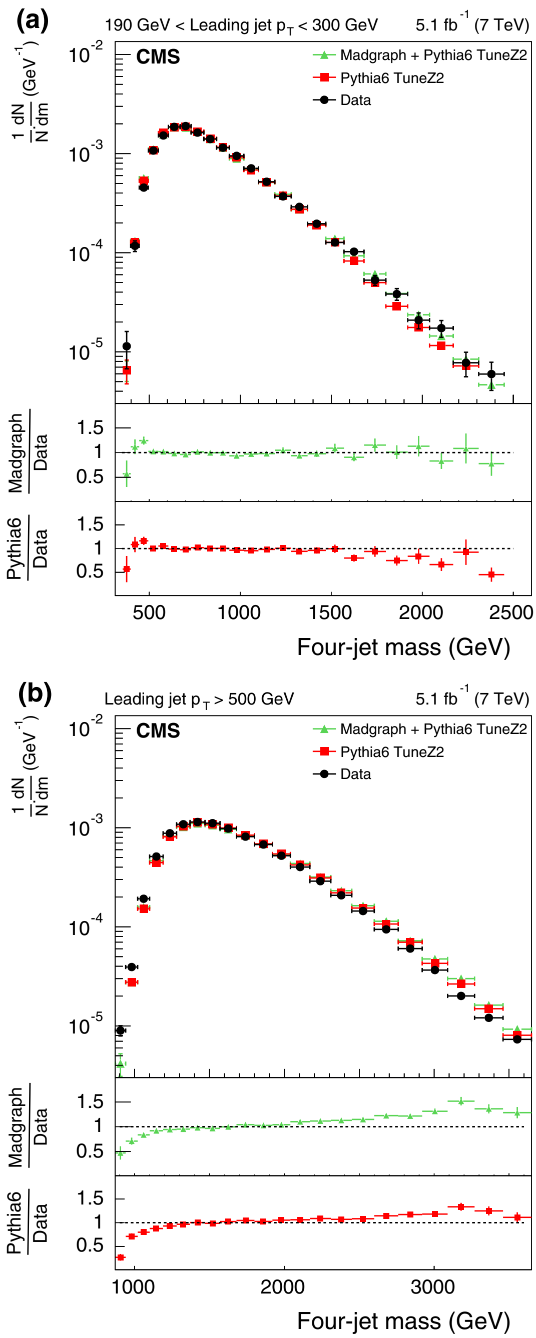

Fig. 4 The *upper panels* display the normalized distributions of the reconstructed four-jet mass for events where the most forward jet has $|y| < 2.5$. The other explanations are the same as Fig. 3

the data. The distributions are presented in this analysis as normalized distributions, thus the absolute scale uncertainty of energy measurement does not play a significant role. There are insignificant contributions due to resolution of y. The main contribution of JES or JER to the uncertainty in the measurements is due to the migration of events from one category of jet multiplicity to the other.

The effect of pileup in the measured distributions has been studied as a function of the number of reconstructed vertices in the event. None of the variables show any significant dependence on the pileup condition, so systematic uncertainty due to pileup can be neglected.

8.1 Jet energy scale

One of the dominant sources of systematic uncertainty is due to the jet energy scale corrections. The JES uncertainty has been estimated to be 2–2.5 % for PF jets [30], depending on the jet p_T and η. In order to map this uncertainty to the multijet variables, all jets in the selected events are systematically shifted by the respective uncertainties, and a new set of values for the multijet variables is calculated. This causes a migration of events from an event category of a given jet multiplicity to a different jet multiplicity. The migration could be as high as 20 % for some of the event categories. The corresponding distributions are then unfolded using the standard procedure as described in Sect. 7. The difference of these values from the central unfolded results is a measure of the uncertainty owing to the JES.

Uncertainties owing to the JES are found to be between 0.2–5.5 % in the three-jet mass, and 0.3–10 % in the four-jet mass. The systematic uncertainties are the largest at both ends of the mass spectra. The systematic uncertainties in scaled energy are between 0.1 and 2.0 %, and those in angular variables are in the range 0.1–3.0 %. There is a small increase in the uncertainty for distributions where there is at least one jet in the endcap region of the detector.

8.2 Jet energy resolution

The JER is measured in data using the p_T balance in dijet events [36]. Based on these measurements, the resolution effects are corrected using simulated events. To study the effect of the difference between the simulated and the measured resolution, several sets of unfolded distributions are obtained using response matrices from the default resolution matrix and changing the jet resolution within its estimated uncertainty. Alternatively, the response matrix is constructed by convolving the generator level distribution with the measured resolution. The measured distribution is unfolded by this response matrix vis-a-vis the response matrix determined using fully simulated sample of PYTHIA6 events. These two estimates provide independent descriptions of the detector modeling and the difference is used as a measure of the systematic uncertainty due to detector performance. Position resolution affects the measurement of the jet direction, and it is estimated using simulated multijet events and validated with data.

Uncertainties owing to the JER are found to be between 0.1–10 % in the three-jet mass, 0.3–15 % in the four-jet mass, 0.1–10 % in the scaled jet energies and 0.2–8.2 % in the angular variables.

8.3 Model dependence in unfolding

Unfolded distributions are obtained using two different response matrices derived from PYTHIA6 and MADGRAPH+PYTHIA6 simulations. The difference in the unfolded values, due to the choice of response functions, gives a measure of the systematic uncertainty. The uncertainties are at the level of 0.1–6.0 % in the three-jet mass, 0.1–3.0 % in the scaled energy distributions of the three-jet variables, 0.1–8.0 % in the four-jet mass and 0.1–6.2 % in the angular variables in the four-jet samples. The uncertainties in the scaled jet energy increases by a few percent for the samples with lower values of leading jet p_T.

Unfolding has been carried out using PYTHIA6 and MADGRAPH + PYTHIA6 samples, which has the same hadronization model. To test the effects of different hadronization models, MC samples from HERWIG++, which provides a different PS and hadronization approach, are used. However, the simulated event sample generated using HERWIG++ is statistically inadequate to be used in a complete unfolding procedure. The difference between bin-by-bin correction factors obtained with PYTHIA6 and HERWIG++ is found to be somewhat larger than the uncertainty due to the difference in the unfolding matrices: 0.1–12 % in the scaled energy distributions of three-jet variables, 0.1–7.7 % in the angular variables in the four-jet samples and 0.1–11.6 % in the jet masses. The larger values from the two estimates are chosen as the systematic uncertainties due to unfolding.

8.4 Event selection

Jet candidates are required to pass certain criteria [37] designed to reduce unwanted detector effects. This analysis uses jets identified with very restrictive criteria on the ratio of the energy carried by neutral to that carried by charged particles. The effect of using these criteria is tested by reevaluating the same distributions with jets selected after relaxing the selection on the fractions of the energy carried by the neutral and the charged particles. Also, the selection on E_T^{miss} is changed, and the effect of this is estimated from the difference in the observed distributions. The uncertainty due to the event selection is found to be below 0.2 %.

8.5 Overall uncertainty

The first three sources mentioned above are the dominant sources of systematic uncertainty. The contributions to the uncertainty from the selection requirements and pileup effects are found to be negligible. The uncertainties are calculated for each bin of the measured distributions and are added in quadrature. The overall systematic uncertainty is found to be smaller than the statistical uncertainty for most of the bins. Typical uncertainties for the six variables studied in this analysis are summarized in Table 3.

Table 3 Uncertainty ranges among the different bins in the topological distributions of the three- and four-jet variables

Uncertainty source	Uncertainty (%) for leading jet p_T	
	190–300 GeV	>500 GeV
Three-jet mass		
Jet and event selection	0.1	0.1
Jet energy scale	0.3–5.0	0.2–5.5
Jet resolution	0.1–10.0	0.2–6.0
Model dependence in unfolding	0.2–11.0	0.2–5.0
Total systematic uncertainty	0.3–12.7	0.2–7.9
Statistical uncertainty	1.4–14.5	0.7–10.2
Scaled energy of the leading jet		
Jet and event selection	0.1	0.1
Jet energy scale	0.1–1.9	0.1–1.4
Jet resolution	0.2–6.2	0.1–5.4
Model dependence in unfolding	0.1–6.0	0.5–3.6
Total systematic uncertainty	0.8–7.2	1.1–5.6
Statistical uncertainty	1.6–17.2	0.6–14.2
Scaled energy of the second-leading jet		
Jet and event selection	0.1	0.1
Jet energy scale	0.1–2.0	0.1–2.0
Jet resolution	0.1–5.0	0.1–4.2
Model dependence in unfolding	0.4–9.0	0.1–3.5
Total systematic uncertainty	1.0–8.3	0.1–4.6
Statistical uncertainty	1.3–16.4	0.9–8.0
Four-jet mass		
Jet and event selection	0.1	0.1
Jet energy scale	0.4–6.9	0.3–7.0
Jet resolution	0.4–11.7	0.2–4.9
Model dependence in unfolding	0.3–7.0	0.5–8.1
Total systematic uncertainty	0.4–13.7	0.5–11.6
Statistical uncertainty	3.1–30.9	1.4–12.5
Bengtsson–Zerwas angle		
Jet and event selection	0.1	0.1
Jet energy scale	0.1–3.0	0.2–2.4
Jet resolution	0.4–5.4	0.2–5.0
Model dependence in unfolding	0.3–3.5	0.1–6.4
Total systematic uncertainty	1.4–5.9	1.0–8.1
Statistical uncertainty	5.1–8.4	2.8–4.0
Nachtmann–Reiter angle		
Jet and event selection	0.1	0.1
Jet energy scale	0.1–1.0	0.1–1.1
Jet resolution	0.1–4.6	0.2–2.1
Model dependence in unfolding	0.2–2.1	0.4–5.0

Table 3 continued

Uncertainty source	Uncertainty (%) for leading jet p_T	
	190–300 GeV	>500 GeV
Total systematic uncertainty	0.9–5.0	0.9–5.2
Statistical uncertainty	3.4–4.2	1.3–1.6

9 Results

9.1 Comparison with models

The normalized differential distributions, corrected for detector effects, are plotted as a function of the three- and four-jet inclusive variables and compared with predictions from the four MC models: PYTHIA6, PYTHIA8, MADGRAPH+PYTHIA6, and HERWIG++. The variables considered for these comparisons are three-jet mass, scaled energies of the leading and next-to-leading jet in the three-jet sample in the three-jet CM frame, four-jet mass, and the two angles χ_{BZ} and θ_{NR}.

For the comparison plots (Figs. 5, 6, 7, 8, 9), the upper panel shows the data and the model predictions with the corresponding statistical uncertainty. For the data, the shaded area shows the statistical and systematic uncertainties added in quadrature. The lower panels in each plot show the ratio of MC prediction to the data for each model. Comparisons are made for two different ranges of the leading jet p_T: $190 < p_T < 300$ GeV and $p_T > 500$ GeV.

Figure 5 shows the normalized corrected differential distribution as a function of the three-jet mass for two ranges of the leading-jet p_T. The three-jet mass distribution broadens for larger p_T thresholds. The models show varying degrees of success for the different ranges of leading-jet p_T. Most models differ from the data in the low-mass spectrum. The PYTHIA6 simulation provides a good description of the data in the lower p_T bin, while it has a larger deviation in the higher p_T bin. The mean difference is at the level of 1.8–4.0 %. Predictions from MADGRAPH + PYTHIA6 and PYTHIA8 agree with the data to within 4.5 %. HERWIG++ provides the worst agreement among the four models – the mean difference is at the level of 4.0–15 %.

Figure 6 shows the corrected normalized differential distribution as a function of the scaled leading-jet energy in the inclusive three-jet sample. The distributions peak close to 1 and the peaks get sharper for higher leading-jet p_T range. The scaled leading-jet energy x_3 is expected to follow a linear rise from $\frac{2}{3}$ to 1 for a phase space model, which has only energy-momentum conservation, while QCD predicts

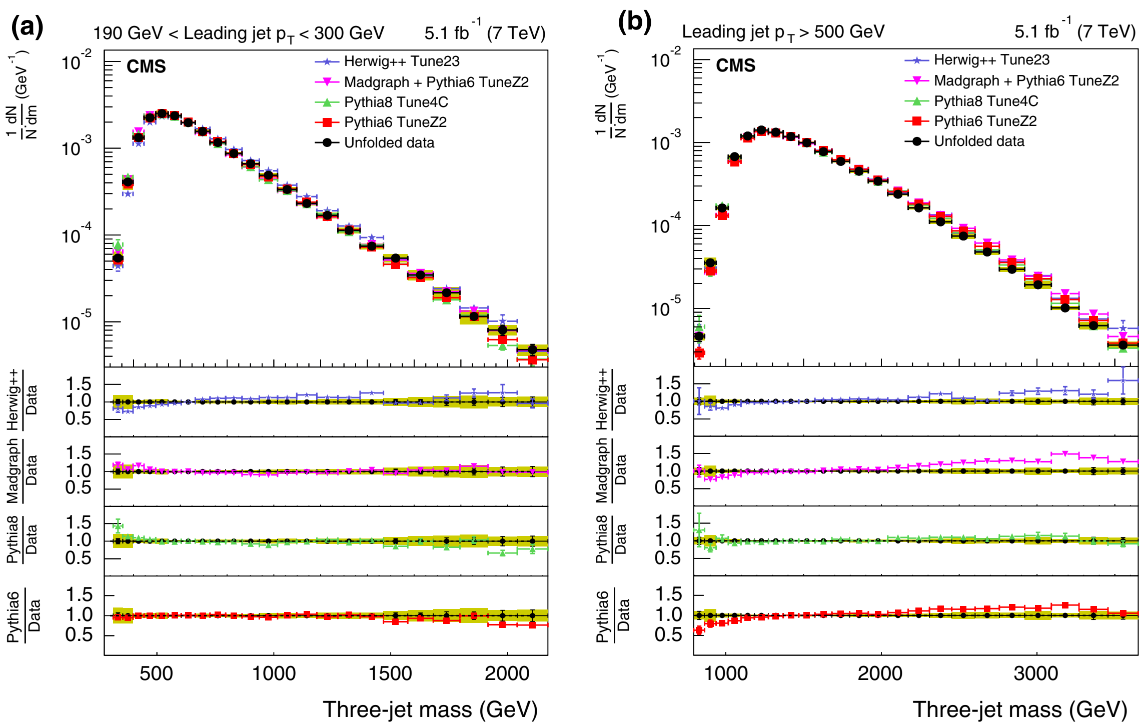

Fig. 5 Distribution of the three-jet mass superposed with predictions from four MC models: PYTHIA6, PYTHIA8, MADGRAPH + PYTHIA6, HERWIG++. The distributions are obtained from inclusive three-jet sample with the jets restricted in the $|y|$ region $0.0 < |y| < 2.5$, and with leading-jet p_T between 190 and 300 GeV (**a**) or above 500 GeV (**b**). The data points are shown with statistical uncertainty only and the bands indicate the statistical and systematic uncertainties combined in quadrature. The *lower panels of each plot* show the ratios of MC predictions to the data. The ratios are shown with statistical uncertainty in the data as well as in the MC, while the *band* shows combined statistical and systematic uncertainties

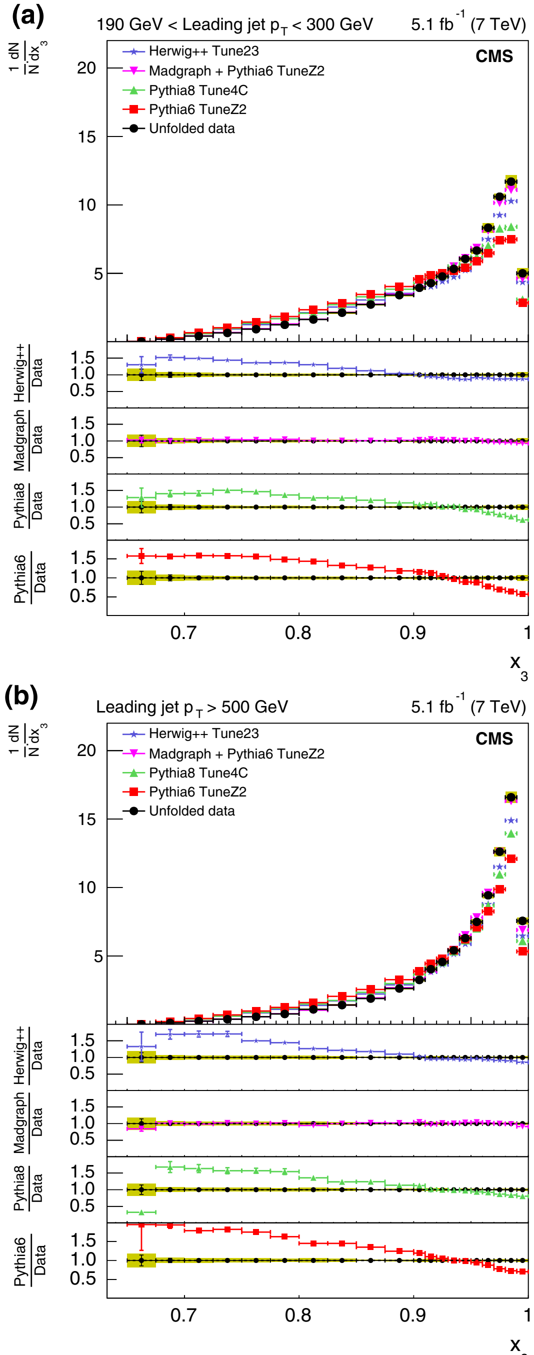

Fig. 6 Corrected normalized distribution of scaled energy of the leading-jet in the inclusive three-jet sample. The other explanations are the same as Fig. 5

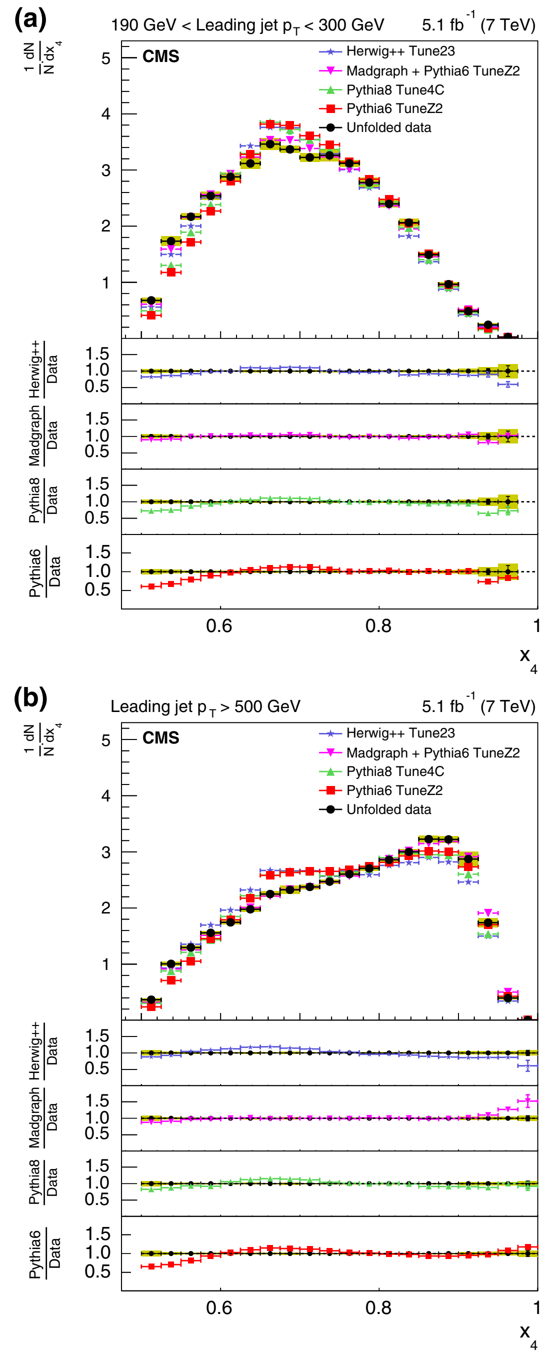

Fig. 7 Corrected normalized distribution of scaled energy of the second-leading jet in the inclusive three-jet sample. The other explanations are the same as Fig. 5

a deviation from linearity at higher values of x_3. This feature is observed in the data, particularly for higher p_T bins. Only MADGRAPH + PYTHIA6 provides a consistent description of the data. The agreement improves for the sample with leading-jet p_T above 500 GeV. The difference between the predictions from MADGRAPH + PYTHIA6 and the data are at the level of 3.5–6.1 %.

Figure 7 shows the corrected normalized differential distribution as a function of the scaled energy of the second-leading jet, x_4, in the inclusive three-jet sample. For kinematic reasons, x_4 is expected to lie between 1/2 and 1. The distribution peaks around 0.65 for the low p_T threshold sample. The peak shifts to higher values of x_4 and the distribution becomes broader for the larger p_T threshold sample. Predic-

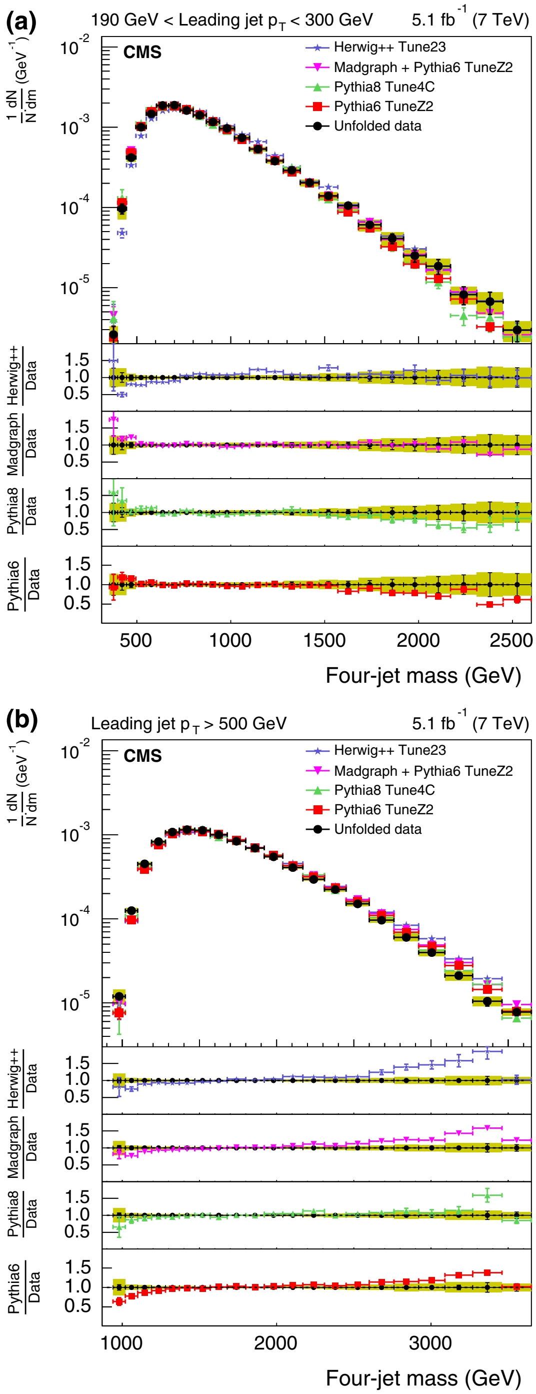

Fig. 8 Corrected normalized distribution of four-jet mass. The other explanations are the same as Fig. 5

tions from MADGRAPH + PYTHIA6 agree with data to within 3.1 %. Predictions from PYTHIA6 as well as PYTHIA8 deviate by as much as 10 % or more from the data. Predictions from HERWIG++ also shows a large deviation at higher p_T bins.

Figure 8 shows comparisons of the corrected normalized differential distribution as a function of the four-jet mass for the four MC models. The distribution broadens at higher minimum p_T value. As can be seen from the figure, HERWIG++ provides the worst comparison. The average deviations are at the level of 15 % for many of the distributions, particularly for the sample with leading-jet p_T between 190 and 300 GeV. The level of agreement for the other three MC models is better than 10 % over the entire p_T region.

The sub-leading jets in the four-jet event category are predominantly due to the secondary splitting of partons. In case of gluon splitting, they can be due to a $q\overline{q}$ pair or gluons. Both the angular distributions, θ_{NR} and χ_{BZ}, are different for these two scenarios and are representative of the colour factors for these couplings.

Figure 9 shows similar comparisons for the Bengtsson–Zerwas angle. Because the azimuthal angle is not defined for the back-to-back jets, the opening angle between the two leading and two nonleading jets is required to be less than 160°. As can be seen from the average deviation of the ratios from unity, predictions from MADGRAPH + PYTHIA6 and HERWIG++ represent the data well, while those from PYTHIA6 do poorly.

Figure 10 shows the corrected normalized differential distribution as a function of the cosine of the Nachtmann–Reiter angle in the inclusive four-jet sample. Most of the models follow the broad features of the data. However, the degree of agreement with data is different among models. MADGRAPH + PYTHIA6 provides the best description of the data; HERWIG++ with angular ordering in the parton shower is close to the data (the agreement is better than 5 %), while PYTHIA6 has the largest deviation (the agreement is typically between 10–12 %).

9.2 Effect of hadronization, underlying event, and PDFs

The disagreement between data and the MC models may arise from the implementation of nonperturbative components in the simulation due to the fragmentation model or the choice of PDF set. These effects have been investigated by studying the uncertainties due to hadronization model and PDF parametrization.

The MC models have different ways of modeling the underlying events and hadronization of the partons into hadrons. This may result in different predictions of the distributions of multijet variables depending on whether they are computed at the hadron or at the parton level. This effect has been investigated by studying two different MC models: PYTHIA6 and HERWIG++. This is done by evaluating the distributions at the parton and hadron level. PYTHIA6 uses the LUND string model, while HERWIG++ uses the cluster model. Also, colour reconnections are done differently in the two models. A generator-level study is carried out for both these models, where the effect of hadronization is studied using distributions from jets at parton- and hadron-level. The ratio of the parton- to the hadron-level distribution is then com-

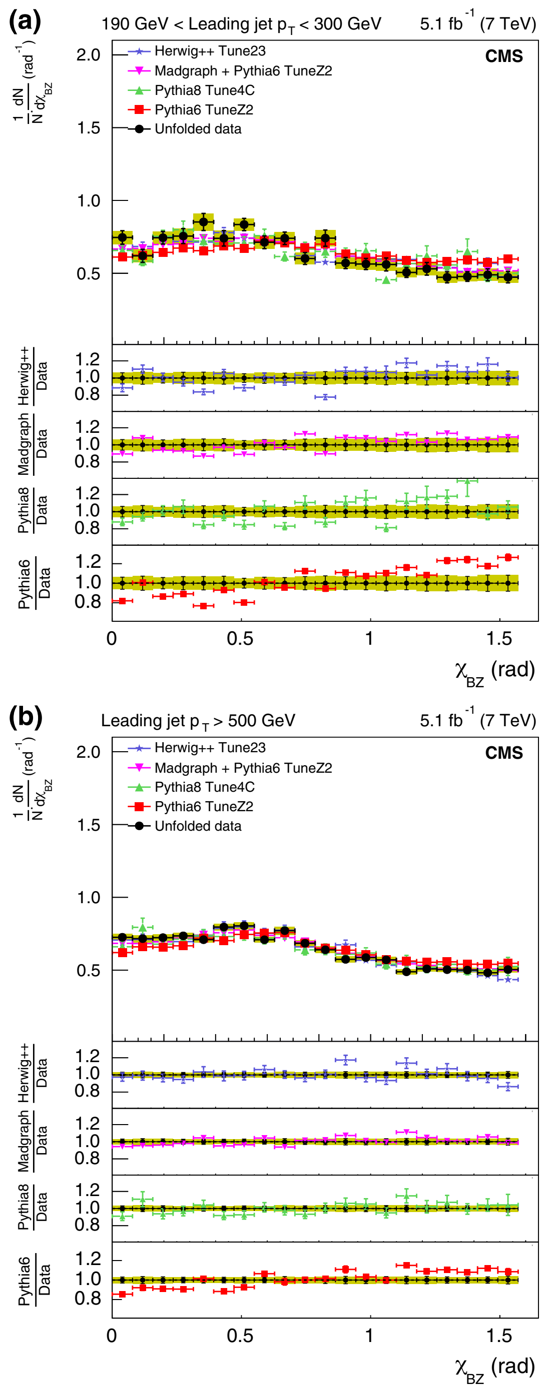

Fig. 9 Corrected normalized distribution of the Bengtsson–Zerwas angle. The other explanations are the same as Fig. 5

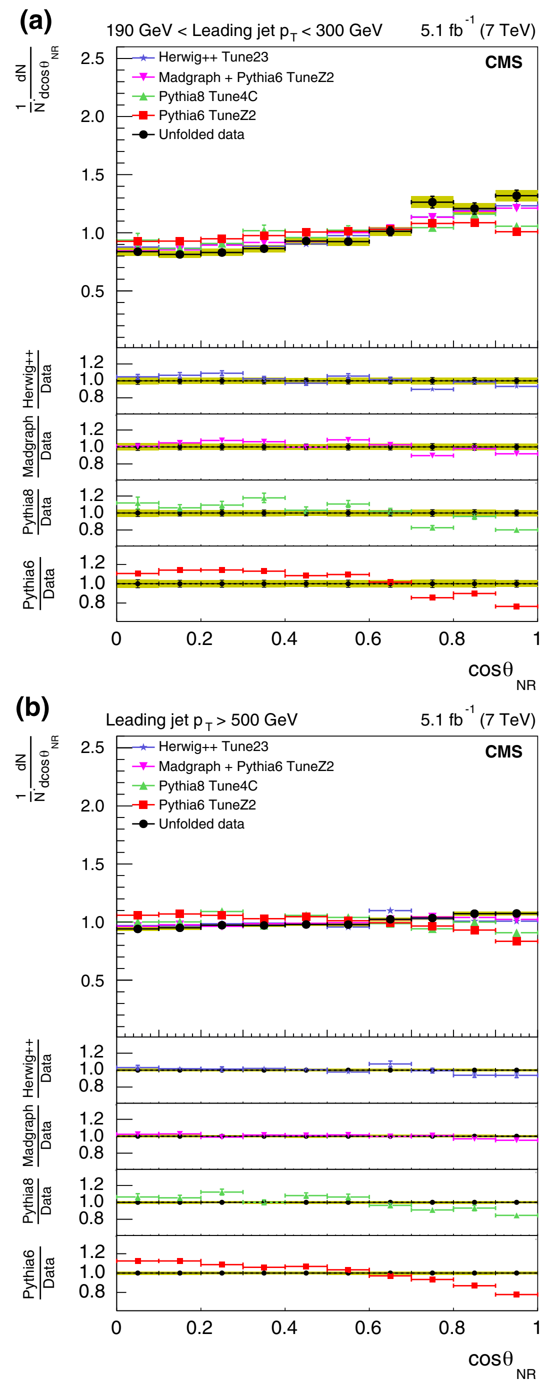

Fig. 10 Corrected normalized distribution of the cosine of the Nachtmann–Reiter angle. The other explanations are the same as Fig. 5

pared. The mean difference between the two hadronization models is typically less than 5 %.

Comparisons are also made to different tunes of the underlying event models within PYTHIA6. The tunes (D6T, DW, P0, Z1, Z2, Z2*) [10,11,38–40] differ in the cutoff used to regularize the $1/p_T^4$ divergence for final-state partons, the ordering of the showers (virtuality ordering vs. p_T ordering), multiparton interaction model, PDFs, and data sets used in the tune. The resulting distributions agree typically within 5 %, so the disagreements with the data cannot be fully explained by this effect.

The MC models use CTEQ6 as the default PDF parametrization. There are many different PDF sets, which are based on different input data, assumptions, and parametrizations. Thus any calculation of a cross section or distributions in the simulation depends on the choice of PDF set.

Also, each PDF set has its own errors from its parametric assumptions and data input to fitting. The effect of the PDF set choice on the multijet variables is calculated according to the recommendation of PDF4LHC group [41,42]. Since comparisons are made only with leading order Monte Carlo models in this paper, only two leading order PDF sets are used in this comparison: CTEQ6l and MSTW2008lo68cl [43]. The uncertainties are found to be typically at the level of 1.0–2.0 % depending on the variable type and p_{T} range considered.

10 Summary

Distributions of topological variables for inclusive three- and four-jet events in pp collisions measured with the CMS detector at a centre-of-mass energy of 7 TeV were presented using a data sample corresponding to an integrated luminosity of 5.1 fb^{-1}. The distributions were corrected for detector effects, and systematic uncertainties were estimated. These corrected distributions were compared with the predictions from four LO MC models: PYTHIA6, PYTHIA8, HERWIG++, and MADGRAPH + PYTHIA6.

Distributions of three- and four-jet invariant mass from all models show significant deviation from the data at high mass. The fact that all models have a common PDF suggests that the PDF errors at high mass are underestimated. The PDFs at high invariant mass have recently been constrained by CMS using dijet p_{T} distributions[44].

The MADGRAPH simulations are based on tree-level calculations for two-, three-, and four-parton final states, while PYTHIA and HERWIG++ can have only two partons in the final state before showering. Not surprisingly, the three-jet predictions of MADGRAPH + PYTHIA6 give a more consistent description of the distributions studied in this analysis. The notable exception is at high x_4 (the next-to-leading jet), where two jets carry most of the CM energy. The difference is probably due to a double counting of three-parton with two-parton (with a parton from showering) final states.

The PYTHIA and HERWIG++ models give poor descriptions of the energy fractions in the three-jet final state. In particular, the distributions of x_3 (the leading jet) show large shape differences between data and theory that are inconsistent with PDFs or hadronization model uncertainties. Since the distributions from MADGRAPH + PYTHIA6 agree with those from the data, the discrepancies with PYTHIA and HERWIG++ are likely due to missing higher multiplicity ME, which are present in MADGRAPH.

All the models compared in this study do remarkably well describing the four-jet Bengtsson–Zerwas angle. The PYTHIA models have some systematic deviation from the data in describing the Nachtmann–Reiter angle. Parton showers with angular ordering, as implemented in HERWIG++, yield a better agreement with the measured data for these angular variables.

Acknowledgments We congratulate our colleagues in the CERN accelerator departments for the excellent performance of the LHC and thank the technical and administrative staffs at CERN and at other CMS institutes for their contributions to the success of the CMS effort. In addition, we gratefully acknowledge the computing centres and personnel of the Worldwide LHC Computing Grid for delivering so effectively the computing infrastructure essential to our analyses. Finally, we acknowledge the enduring support for the construction and operation of the LHC and the CMS detector provided by the following funding agencies: the Austrian Federal Ministry of Science, Research and Economy and the Austrian Science Fund; the Belgian Fonds de la Recherche Scientifique, and Fonds voor Wetenschappelijk Onderzoek; the Brazilian Funding Agencies (CNPq, CAPES, FAPERJ, and FAPESP); the Bulgarian Ministry of Education and Science; CERN; the Chinese Academy of Sciences, Ministry of Science and Technology, and National Natural Science Foundation of China; the Colombian Funding Agency (COLCIENCIAS); the Croatian Ministry of Science, Education and Sport, and the Croatian Science Foundation; the Research Promotion Foundation, Cyprus; the Ministry of Education and Research, Estonian Research Council via IUT23-4 and IUT23-6 and European Regional Development Fund, Estonia; the Academy of Finland, Finnish Ministry of Education and Culture, and Helsinki Institute of Physics; the Institut National de Physique Nucléaire et de Physique des Particules/CNRS, and Commissariat à l'Énergie Atomique et aux Énergies Alternatives/CEA, France; the Bundesministerium für Bildung und Forschung, Deutsche Forschungsgemeinschaft, and Helmholtz-Gemeinschaft Deutscher Forschungszentren, Germany; the General Secretariat for Research and Technology, Greece; the National Scientific Research Foundation, and National Innovation Office, Hungary; the Department of Atomic Energy and the Department of Science and Technology, India; the Institute for Studies in Theoretical Physics and Mathematics, Iran; the Science Foundation, Ireland; the Istituto Nazionale di Fisica Nucleare, Italy; the Ministry of Science, ICT and Future Planning, and National Research Foundation (NRF), Republic of Korea; the Lithuanian Academy of Sciences; the Ministry of Education, and University of Malaya (Malaysia); the Mexican Funding Agencies (CINVESTAV, CONACYT, SEP, and UASLP-FAI); the Ministry of Business, Innovation and Employment, New Zealand; the Pakistan Atomic Energy Commission; the Ministry of Science and Higher Education and the National Science Centre, Poland; the Fundação para a Ciência e a Tecnologia, Portugal; JINR, Dubna; the Ministry of Education and Science of the Russian Federation, the Federal Agency of Atomic Energy of the Russian Federation, Russian Academy of Sciences, and the Russian Foundation for Basic Research; the Ministry of Education, Science and Technological Development of Serbia; the Secretaría de Estado de Investigación, Desarrollo e Innovación and Programa Consolider-Ingenio 2010, Spain; the Swiss Funding Agencies (ETH Board, ETH Zurich, PSI, SNF, UniZH, Canton Zurich, and SER); the Ministry of Science and Technology, Taipei; the Thailand Center of Excellence in Physics, the Institute for the Promotion of Teaching Science and Technology of Thailand, Special Task Force for Activating Research and the National Science and Technology Development Agency of Thailand; the Scientific and Technical Research Council of Turkey, and Turkish Atomic Energy Authority; the National Academy of Sciences of Ukraine, and State Fund for Fundamental Researches, Ukraine; the Science and Technology Facilities Council, UK; the US Department of Energy, and the US National Science Foundation. Individuals have received support from the Marie-Curie programme and the European Research Council and EPLANET (European Union); the Leventis Foundation; the A. P. Sloan Foundation; the Alexander von Humboldt Foundation; the Belgian Federal Science Policy Office; the Fonds pour la Formation à la Recherche dans l'Industrie et dans l'Agriculture

(FRIA-Belgium); the Agentschap voor Innovatie door Wetenschap en Technologie (IWT-Belgium); the Ministry of Education, Youth and Sports (MEYS) of the Czech Republic; the Council of Science and Industrial Research, India; the HOMING PLUS programme of Foundation for Polish Science, cofinanced from European Union, Regional Development Fund; the Compagnia di San Paolo (Torino); the Consorzio per la Fisica (Trieste); MIUR Project 20108T4XTM (Italy); the Thalis and Aristeia programmes cofinanced by EU-ESF and the Greek NSRF; and the National Priorities Research Program by Qatar National Research Fund.

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