

Search for contact interactions using the inclusive jet p_T spectrum in pp collisions at $\sqrt{s} = 7$ TeV

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Abstract

Results are reported of a search for a deviation in the jet production cross section from the prediction of perturbative quantum chromodynamics at next-to-leading order. The search is conducted using a 7 TeV proton-proton data sample corresponding to an integrated luminosity of 5.0 fb^{-1} , collected with the Compact Muon Solenoid detector at the Large Hadron Collider. A deviation could arise from interactions characterized by a mass scale Λ too high to be probed directly at the LHC. Such phenomena can be modeled as contact interactions. No evidence of a deviation is found. Using the CL_s criterion, lower limits are set on Λ of 9.9 TeV and 14.3 TeV at 95% confidence level for models with destructive and constructive interference, respectively. Limits obtained with a Bayesian method are also reported.

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1 Introduction

Interactions at an energy scale much lower than the mass of the mediating particle can be modeled by contact interactions (CI) [1–4] governed by a single mass scale conventionally denoted by Λ . A search for contact interactions is therefore a search for interactions whose detailed characteristics become manifest only at higher energies. Contact interactions can affect the jet angular distributions as well as the jet transverse momentum (p_T) spectra, particularly for low-rapidity jets. Lower limits on Λ have been set by the CDF [5], D0 [6], and ATLAS [7] collaborations. The Compact Muon Solenoid (CMS) collaboration has previously measured the dijet angular distribution [8] using a data set of $\sqrt{s} = 7$ TeV proton-proton collisions corresponding to an integrated luminosity of 2.2 fb^{-1} , and found $\Lambda > 8.4$ TeV and $\Lambda > 11.7$ TeV at 95% confidence level (CL), for models with destructively and constructively interfering amplitudes, respectively.

The inclusive jet p_T spectrum, i.e., the spectrum of jets in $p + p \rightarrow \text{jet} + X$ events, where X can be any collection of particles, is generally considered to be less sensitive to the presence of contact interactions than the jet angular distribution. This perception is due to the jet p_T spectrum's greater dependence on the jet energy scale (JES) and on the parton distribution functions (PDF), which are difficult to determine accurately. However, considerable progress has been made by the CMS collaboration in understanding the JES [9]. The understanding of PDFs has also improved greatly at high parton momentum fraction [10–12], in part because of the important constraints on the gluon PDF provided by measurements at the Tevatron [13, 14]. These developments have made the jet p_T spectrum a competitive observable to search for phenomena described by contact interactions, reprising the method that was used in searches by CDF [15] and D0 [16].

In this paper, we report the results of a search for a deviation in the jet production cross section from the next-to-leading-order (NLO) quantum chromodynamics (QCD) prediction of jets produced at low-rapidity with transverse momenta >500 GeV. The analysis is based on a 7 TeV proton-proton data sample corresponding to an integrated luminosity of 5.0 fb^{-1} , collected with the CMS detector at the Large Hadron Collider (LHC).

2 Theoretical models

The experimental results are interpreted in terms of a CI model described by the effective Lagrangian [3, 17]

$$L = \zeta \frac{2\pi}{\Lambda^2} (\bar{q}_L \gamma^\mu q_L) (\bar{q}_L \gamma_\mu q_L), \quad (1)$$

where q_L denotes a left-handed quark field and $\zeta = +1$ or -1 for destructively or constructively interfering amplitudes, respectively. The amplitude for jet production can be written as

$$a = a_{\text{SM}} + \lambda a_{\text{CI}}$$

where a_{SM} and a_{CI} are the standard model (SM) and contact interaction amplitudes, respectively. Since the amplitude is linear in $\lambda = 1/\Lambda^2$, the cross section σ_k in the k th jet p_T bin is given by

$$\sigma_k = c_k + b_k \lambda + a_k \lambda^2, \quad (2)$$

where c_k , b_k , and a_k are jet- p_T -dependent coefficients.

We use models characterized by the cross section $\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)$, where $\text{QCD}_{\text{NLO}} = c_k$ is the inclusive jet cross section computed at next-to-leading order, and $\text{CI}(\Lambda) = b_k \lambda + a_k \lambda^2$ parame-

terizes the deviation of the inclusive jet cross section from the QCD prediction arising from the hypothesized contact interactions. The QCD_{NLO} cross section is calculated with version 2.1.0-1062 of the fastNLO program with scenario table fnl2332y0.tab [18] using the NLO CTEQ6.6 PDFs [19]. We do not unfold the observed inclusive jet p_T spectrum. Instead, the NLO QCD jet p_T spectrum is convolved with the CMS jet response function, where the jet energy resolution (JER) σ_{p_T} for low-rapidity jets is given by

$$\sigma_{p_T} = p_T \sqrt{-\frac{n^2}{p_T^2} + \frac{s^2 p_T^m}{p_T} + c^2}, \quad (3)$$

with $n = 5.09$, $s = 0.512$, $m = 0.325$, $c = 0.033$, and compared directly with the observed spectrum using a likelihood function. Equation (3) is the standard form for the calorimeter resolution function, modified to account for a weak p_T dependence of the coefficient of the (p_T^{-1}) stochastic term and to model better the resolution of low p_T jets by using a negative coefficient for the (p_T^{-2}) noise term. For brevity, we shall refer to the smeared spectrum as the NLO QCD jet p_T spectrum.

The signal term $\text{CI}(\Lambda)$ is modeled by subtracting the leading-order (LO) QCD jet cross section (QCD_{LO}) from the LO jet cross section computed with a contact term. The leading-order jet p_T spectra are computed by generating events with and without a CI term using the program PYTHIA 6.422, the Z2 underlying event tune [17, 20], and the same CTEQ PDFs used to calculate QCD_{NLO} . The generated events are processed with the full CMS detector simulation program, based on GEANT4 [21]. Interactions between all quarks are included (Appendix A) and we consider models both with destructive and constructive interference between the QCD and CI amplitudes. We note that NLO corrections to the contact interaction model have recently become available [22], and we plan to use these results in future studies. These corrections are expected to change the results by less than 5%.

The jet p_T dependence of $\text{CI}(\Lambda)$ is modeled by fitting the ratio $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)]/\text{QCD}_{\text{NLO}}$ simultaneously to four PYTHIA CI models with $\Lambda = 3, 5, 8$, and 12 TeV. The fit is performed in this manner in order to construct a smooth interpolation over the four cross section ratios. Several functional forms were investigated that gave satisfactory fits, including the ansatz [23]:

$$f = 1 + p_1 \left(\frac{p_T}{100 \text{ GeV}} \right)^{p_2} \left(\frac{\lambda}{1 \text{ TeV}^{-2}} \right) + p_3 \left(\frac{p_T}{100 \text{ GeV}} \right)^{p_4} \left(\frac{\lambda}{1 \text{ TeV}^{-2}} \right)^2. \quad (4)$$

In a generator-level study, we verified the adequacy of the extrapolation of Eq. (4) up to 25 TeV. The results of fitting Eq. (4) to models with destructive interference are shown in Figure 1. The fit shown in Fig. 1 uses the central values of the JES, JER, and PDF parameters and the renormalization (μ_r) and factorization (μ_f) scales set to $\mu_r = \mu_f = \text{jet } p_T$. Models with constructive interference are obtained by reversing the sign of the parameter p_1 . The fit parameters are given in Table 1. Figures 2 and 3 show model spectra in the jet p_T range $500 \leq p_T \leq 2000 \text{ GeV}$ for values of Λ that are close to the limits reported in this paper. Figure 2 shows that the jet production cross section is enhanced at sufficiently high jet p_T . However, for interactions that interfere destructively, the cross section can decrease relative to the NLO QCD prediction. For example, for $\Lambda = 10 \text{ TeV}$, the $\text{QCD}_{\text{NLO}} + \text{CI}$ cross section is lower than the QCD_{NLO} cross section for jet $p_T < 1.3 \text{ TeV}$. Figure 3 shows the contact p interaction signal, $\text{CI}(\Lambda)$, as a function of jet p_T .

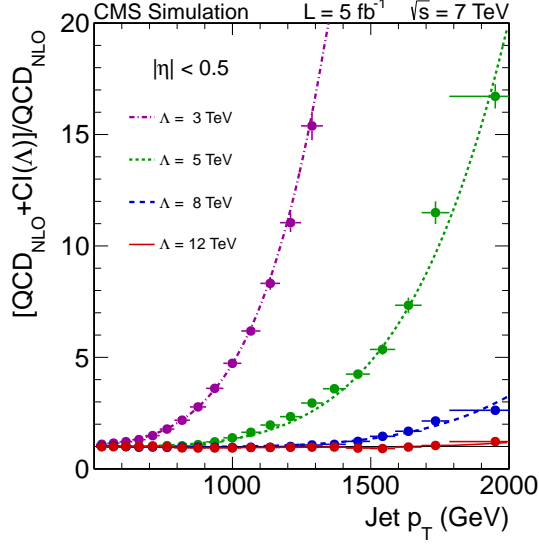


Figure 1: The cross section ratios, $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)]/\text{QCD}_{\text{NLO}}$, with $\Lambda = 3, 5, 8,$ and 12 TeV. The points with error bars are the theoretical values of the cross section ratios. The curves are the results of a fit of Eq. (4) simultaneously to the four cross section ratios. The NLO QCD jet p_T spectrum is calculated using the nominal values of the JES, JER, PDF, renormalization and factorization scales for models with destructive interference. The values of the parameters of the fit are given in Table 1.

Table 1: The fit parameters associated with Fig. 1. The first row lists the values of the parameters $p_1, p_2, p_3,$ and p_4 , while the remaining rows list the elements of the associated covariance matrix.

	p_1	p_2	p_3	p_4
	-1.5×10^{-3}	3.6	1.9×10^{-3}	5.2
p_1	1.4×10^{-6}	3.6×10^{-4}	-3.4×10^{-7}	6.8×10^{-5}
p_2	3.6×10^{-4}	9.2×10^{-2}	-8.4×10^{-5}	1.7×10^{-2}
p_3	-3.4×10^{-7}	-8.4×10^{-5}	1.0×10^{-7}	-2.0×10^{-5}
p_4	6.8×10^{-5}	1.7×10^{-2}	-2.0×10^{-5}	4.1×10^{-3}

3 Experimental setup

The CMS coordinate system is right-handed with the origin at the center of the detector, the x axis directed toward the center of the LHC ring, the y axis directed upward, and the z axis directed along the counterclockwise proton beam. We define ϕ to be the azimuthal angle, θ to be the polar angle, and the pseudorapidity to be $\eta \equiv -\ln[\tan(\theta/2)]$. The central feature of the CMS apparatus is a superconducting solenoid of 6 m internal diameter, operating with a magnetic field strength of 3.8 T. Within the field volume are the silicon pixel and strip trackers and the barrel and endcap calorimeters with $|\eta| < 3$. Outside the field volume, in the forward region, there is an iron/quartz-fiber hadron calorimeter ($3 < |\eta| < 5$). Further details about the CMS detector may be found elsewhere [24].

Jets are built from the five types of reconstructed particles: photons, neutral hadrons, charged hadrons, muons, and electrons, using the CMS particle-flow reconstruction method [25] and the anti- k_T algorithm with a distance parameter of 0.7 [26–28]. The jet energy scale correction is derived as a function of the jet p_T and η , using a p_T -balancing technique [9], and applied to

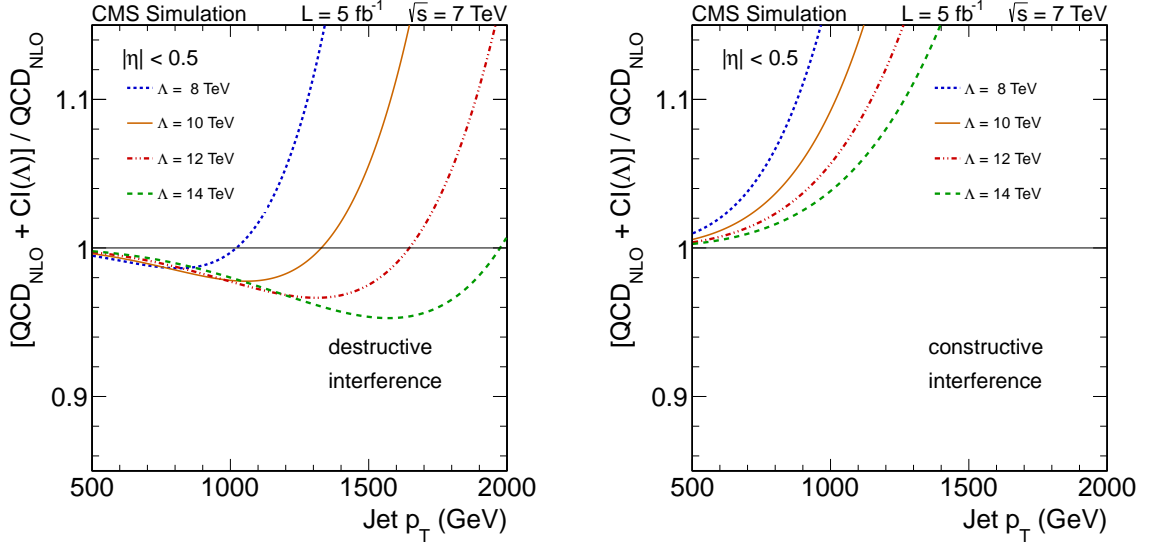


Figure 2: The cross section ratios, $f = [\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)] / \text{QCD}_{\text{NLO}}$, with $\Lambda = 8, 10, 12$, and 14 TeV, for models with destructive (left) and constructive (right) interference.

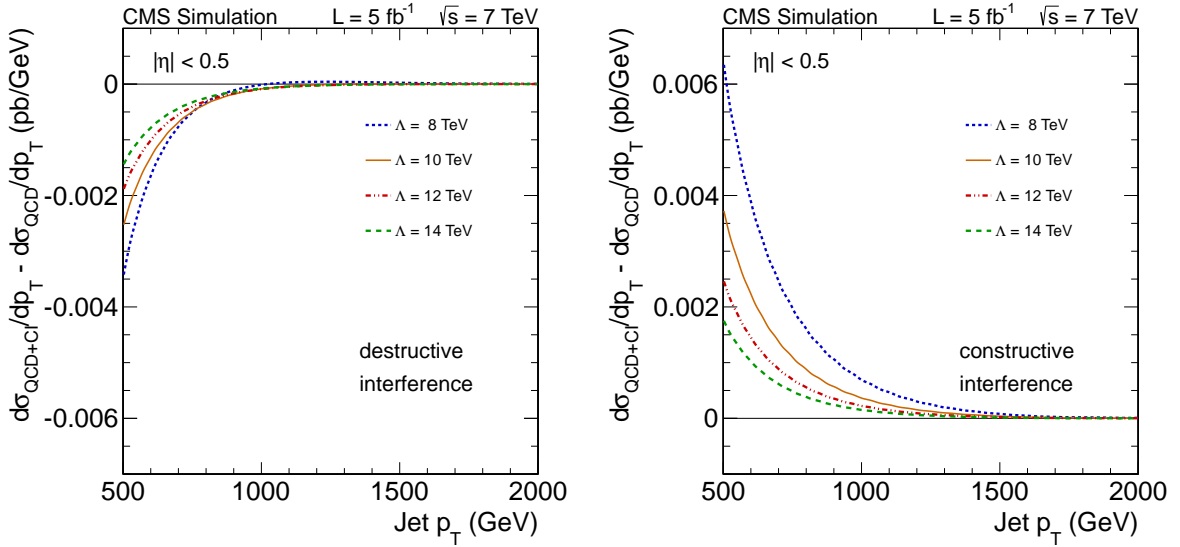


Figure 3: The CI signal spectra, defined as $d\sigma_{\text{QCD}+\text{CI}}/dp_T - d\sigma_{\text{QCD}}/dp_T$ (pb/GeV) with $\Lambda = 8, 10, 12$ and 14 TeV, for models with destructive (left) and constructive (right) interference.

all components of the jet four momentum.

The results reported are based on data collected using un-prescaled single-jet triggers with p_T thresholds that were changed in steps from 240 to 300 GeV during the data-taking period. The trigger thresholds were changed in response to the increase in instantaneous luminosity. The jet trigger efficiency is constant, $\sim 98.8\%$, above ~ 400 GeV, well below the search region. Events with hadron calorimeter noise are removed [29] and each selected event must have a primary vertex within 24 cm of the geometric center of the detector along the z axis and within 0.2 cm in the transverse x - y plane, defined by criteria described in [30]. The search is restricted to $|\eta| < 0.5$ where the effects of contact interactions are predicted to be the largest [1–4]. The jet

p_T spectrum is divided into 20 p_T bins in the search region $507 \leq p_T \leq 2116$ GeV, where the bin width is approximately equal to the jet resolution σ_{p_T} given in Eq. (3). No jets are observed above 2000 GeV transverse energy.

4 Results

In Figure 4 we compare the observed inclusive jet p_T spectrum with the NLO QCD jet p_T spectrum, which is normalized to the total observed jet count in the search region using the normalization factor 4.007 ± 0.009 (stat.) fb^{-1} (Section 5). The normalization is the ratio of the observed jet count to the predicted cross section in the search region. The data and the prediction are in good agreement as indicated by two standard criteria, the Kolmogorov-Smirnov probability $\text{Pr}(\text{KS})$ of 0.66 and the χ^2 per number of degrees of freedom (NDF) of 23.5/19. Table 2 lists the observed jet counts. Figure 5 compares the observed jet p_T spectrum in the search region with model spectra for different values of Λ , for models with destructive interference. Figure 6 compares the data with models with constructive interference.

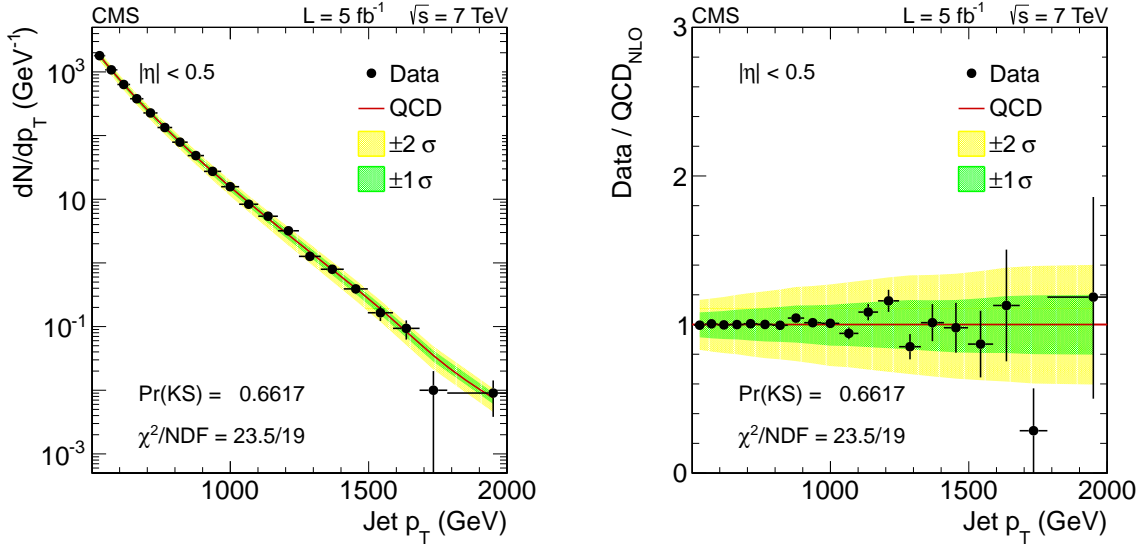


Figure 4: The observed jet p_T spectrum compared with the NLO QCD jet p_T spectrum (left). The bands represent the total uncertainty in the prediction and incorporate the uncertainties in the PDFs, jet energy scale, jet energy resolution, the renormalization and factorization scales, and the modeling of the jet p_T dependence of the parameters in Eq. (4). The ratio of the observed to the predicted spectrum (right). The error bars represent the statistical uncertainties in the expected bin count.

5 Statistical analysis

Since there are no significant deviations between the observed and predicted spectra, the results are interpreted in terms of lower limits on the CI scale Λ using the models described in Section 2. The dominant sources of systematic uncertainties are associated with the JES, the PDFs, the JER, the renormalization (μ_r) and factorization (μ_f) scales, and the modeling parameters of Eq. (4). Non-perturbative corrections are less than 1% for transverse momenta above ~ 400 GeV [30], are negligible compared with other uncertainties, and are therefore not applied to our analysis.

Table 2: The observed jet count for each jet p_T bin in the range 507–2116 GeV.

Bin	p_T (GeV)	Jets	Bin	p_T (GeV)	Jets
1	507–548	73792	11	1032–1101	576
2	548–592	47416	12	1101–1172	384
3	592–638	29185	13	1172–1248	243
4	638–686	18187	14	1248–1327	100
5	686–737	11565	15	1327–1410	66
6	737–790	7095	16	1410–1497	34
7	790–846	4413	17	1497–1588	15
8	846–905	2862	18	1588–1684	9
9	905–967	1699	19	1684–1784	1
10	967–1032	1023	20	1784–2116	3

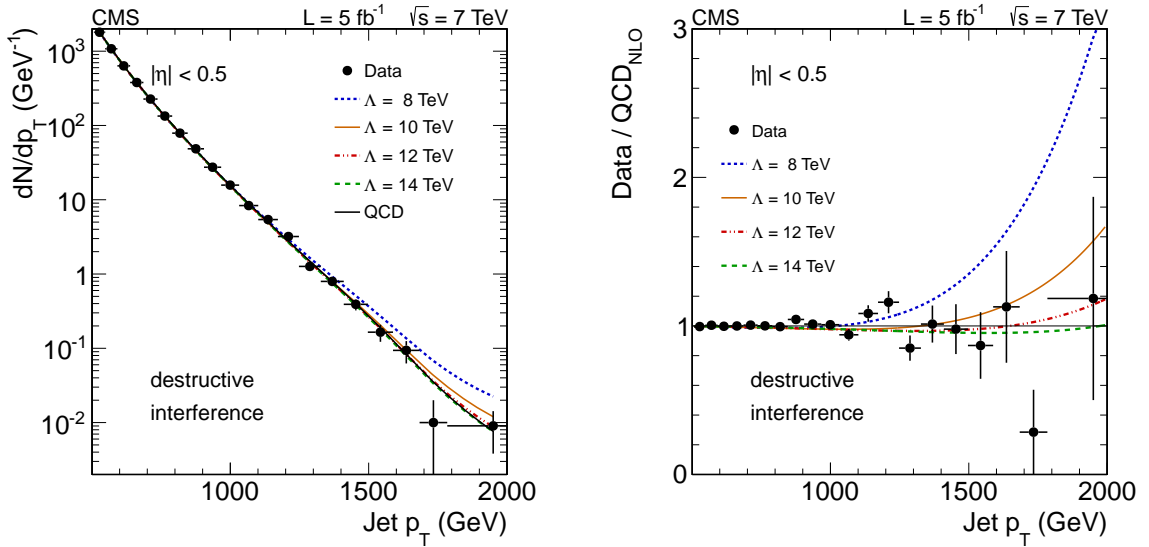


Figure 5: The data compared with model spectra for different values of Λ for models with destructive interference (left). The ratio of these spectra to the NLO QCD jet p_T spectrum (right).

In the search region, the inclusive jet spectrum has a range of five orders of magnitude, which causes the limits on Λ to be sensitive to the choice of the normalization factor and the size of the data sets. We have found that a few percent change in the normalization factor can cause limits to change by as much as 50%. Therefore, for the purpose of computing limits, we have chosen to sidestep the issue of normalization by considering only the shape of the jet p_T spectrum. This we achieve by using a multinomial distribution, which is the probability to observe K counts, N_j , $j = 1, \dots, K$, given the observation of a total count $N = \sum_{j=1}^K N_j$. The likelihood is then defined by

$$p(D|\lambda, \omega) = \frac{N!}{N_1! \dots N_K!} \prod_{j=1}^K \left(\frac{\sigma_j}{\sigma} \right)^{N_j}, \quad (5)$$

where $K = 20$ is the number of bins in the search region, N_j is the jet count in the j th jet p_T bin, $D \equiv N_1, \dots, N_K$, $\sigma = \sum_{j=1}^K \sigma_j$ and N are the total cross section and total observed count, respectively, in the search region, and the symbol ω denotes the nuisance parameters p_1, \dots, p_4 in Eq. (4).

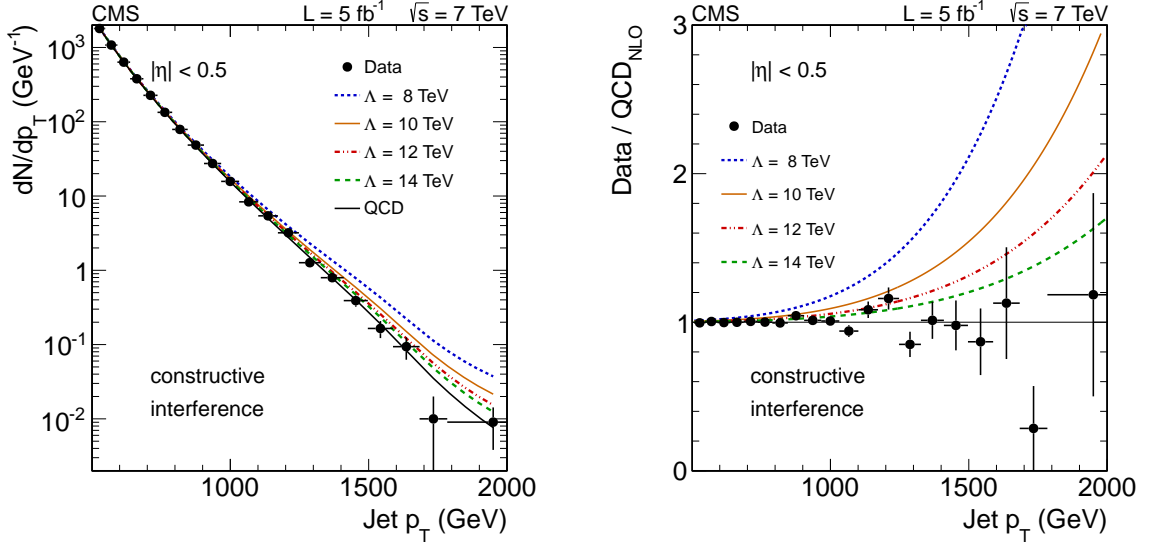


Figure 6: The data compared with model spectra for different values of Λ for models with constructive interference (left). The ratio of these spectra to the NLO QCD jet p_T spectrum (right).

We account for systematic uncertainties by integrating the likelihood with respect to a nuisance prior $\pi(\omega)$. In practice, the likelihood is averaged over the nuisance parameters, ω , using a discrete representation of the prior $\pi(\omega)$ constructed as described in Section 5.1. This calculation yields the marginal likelihood $p(D|\lambda) \approx \frac{1}{M} \sum_{m=1}^M p(D|\lambda, \omega_m)$, where M is the number of points sampled from the nuisance prior $\pi(\omega)$ described in Appendix B.1, which is the basis of the limit calculations. The likelihood functions for models with destructive and constructive interference are shown in Figure 7.

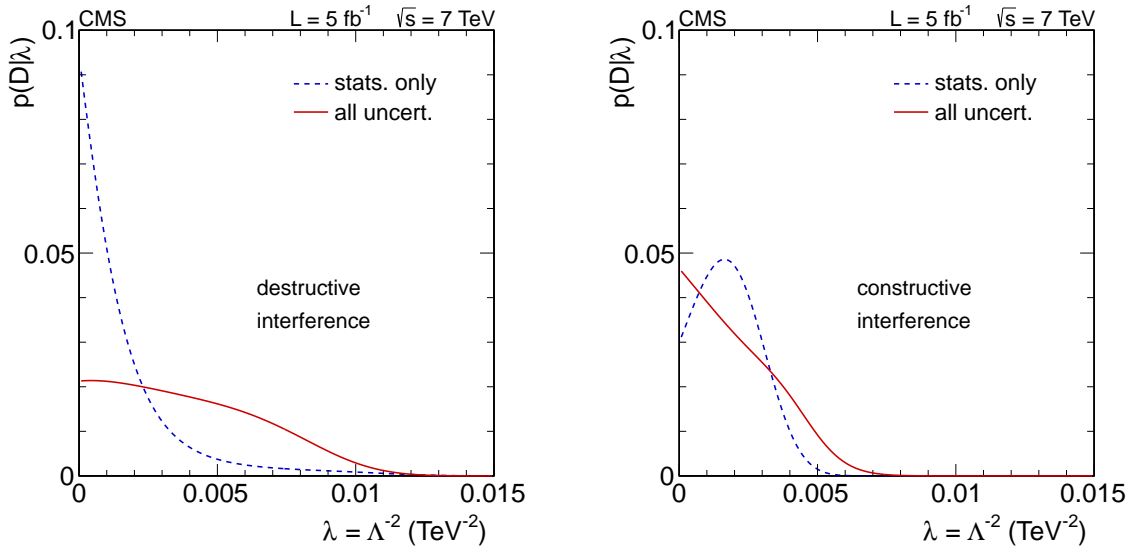


Figure 7: The likelihood functions assuming a model with either destructive (left) or constructive (right) interference. The dashed curve is the likelihood function including statistical uncertainties only and the central values of all nuisance parameters. The solid curve is the likelihood marginalized over all systematic uncertainties.

5.1 Uncertainties

In principle, a discrete representation of the nuisance prior $\pi(\omega)$ can be constructed by sampling simultaneously the JES, JER, PDFs, and the three values of μ_f and μ_r : $p_T/2$, p_T , and $2p_T$. However, the CTEQ collaboration [19] does not provide a sampling of PDFs. Instead, CTEQ6.6 contains 44 PDF sets in which the 22 PDF parameters are shifted by approximately ± 1.64 standard deviations. If we assume the Gaussian approximation to be valid, we can construct approximate 20×20 covariance matrices for the jet spectra from the 44 PDF sets. Using these matrices, we generate ensembles of six correlated spectra: QCD_{NLO} , QCD_{LO} , and $(\text{QCD} + \text{CI}(\Lambda))_{\text{LO}}$ with $\Lambda = 3, 5, 8$, and 12 TeV. The generation is performed for models both with destructive and constructive interference. The details of our procedure, which also includes simultaneous sampling of the JES and JER parameters, are given in Appendix B.1.

For a given set of values for the JES, JER, PDF, μ_r , and μ_f parameters, Eq. (4) is fitted to the ratio $(\text{QCD}_{\text{NLO}} + \text{CI})/\text{QCD}_{\text{NLO}}$ simultaneously to the four models with $\Lambda = 3, 5, 8$, and 12 TeV. We then sample a single set of the four nuisance parameters $\omega = p_1, p_2, p_3, p_4$ from a multivariate Gaussian using the fitted values and the associated 4×4 covariance matrix. The sampling and fitting procedure is repeated 500 times, thereby generating a discrete representation of the nuisance prior $\pi(\omega)$ that incorporates all uncertainties. We have verified that our conclusions are robust with respect to variations in the size of the sample that represents $\pi(\omega)$.

5.2 Lower limits on Λ

We use the CL_s criterion [31, 32] to compute upper limits on λ . For completeness, we give the details of these calculations in Appendix B.2. Using the procedure described in the Appendix, we obtain 95% lower limits on Λ of 9.9 TeV and 14.3 TeV for models with destructive and constructive interference, respectively. These more stringent limits supersede those published by CMS based on a measurement of the dijet angular distribution [8]. The current search is more sensitive than the earlier dijet search as evidenced by the expected limits, which for this analysis are 9.5 ± 0.6 TeV and 13.6 ± 1.6 TeV, respectively, obtained using 5 fb^{-1} of data.

Limits are also computed with a Bayesian method (Appendix B.3) using the marginal likelihood $p(D|\lambda)$ and two different priors for λ : a prior flat in λ and a reference prior [33–35]. Using a flat prior, we find lower limits on Λ of 10.6 TeV and 14.6 TeV at 95% confidence level for models with destructive and constructive interference, respectively. The corresponding limits using the reference prior are 10.1 TeV and 14.1 TeV at 95% confidence level, respectively.

6 Summary

The inclusive jet p_T spectrum of 7 TeV proton-proton collision events in the ranges $507 \leq p_T \leq 2116 \text{ GeV}$ and $|\eta| < 0.5$ has been studied using a data set corresponding to an integrated luminosity of 5.0 fb^{-1} . The observed jet p_T spectrum is found to be in agreement with the jet p_T spectrum predicted using perturbative QCD at NLO when the predicted spectrum is convolved with the CMS jet response function and normalized to the observed spectrum in the search region. Should additional interactions exist that can be modeled as contact interactions with either destructive or constructive interference, their scale Λ is above 9.9 TeV and 14.3 TeV, respectively, at 95% confidence level. We plan to extend this study to the full 8 TeV CMS data set, making use of a recently released program [36] to calculate at next-to-leading order the inclusive jet p_T spectrum with contact interactions.

It is noteworthy that the limits reported in this paper, which are the most sensitive limits pub-

lished to date, have been obtained reprising the classic method to search for contact interactions: namely, searching for deviations from QCD at high jet transverse momentum.

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A PYTHIA 6.422 contact interaction configuration

The scale Λ is defined by the CI model in PYTHIA. In order to facilitate the re-interpretation of the results using a different model, we provide the details of the PYTHIA configuration in Table 3 for $\Lambda = 8$ TeV and final state parton transverse momenta, \hat{p}_T , in the range $170 \leq \hat{p}_T \leq 230$ GeV.

Table 3: PYTHIA 6.422 configuration for $\Lambda = 8$ TeV contact interactions.

PYTHIA 6.422 settings specific to contact interactions	
Settings	Description
ITCM(5)=2	Switch on contact int. for all quarks
RTCM(41)=8000	Set contact scale Λ to 8 TeV
RTCM(42)=1	Sign of contact int. is +
MSUB(381)=1	$q_i q_j \rightarrow q_i q_j$ via QCD plus a contact int.
MSUB(382)=1	$q_i \bar{q}_i \rightarrow q_k \bar{q}_k$ via QCD plus a contact int.
MSUB(13)=1	$q_i \bar{q}_i \rightarrow gg$ via normal QCD
MSUB(28)=1	$q_i g \rightarrow q_i g$ via normal QCD
MSUB(53)=1	$gg \rightarrow q_k \bar{q}_k$ via normal QCD
MSUB(68)=1	$gg \rightarrow gg$ via normal QCD
CKIN(3)=170	minimum \hat{p}_T for hard int.
CKIN(4)=230	maximum \hat{p}_T for hard int.

B Statistical details

B.1 Nuisance prior

We approximate the nuisance prior $\pi(\omega)$ starting with two sets of ensembles. In the first, the six 20-bin model spectra QCD_{NLO} , QCD_{LO} , and $[\text{QCD} + \text{CI}(\Lambda)]_{\text{LO}}$ with $\Lambda = 3, 5, 8,$ and 12 TeV are varied, reflecting random variations in the PDF parameters as well as random choices of the three μ_r and μ_f scales, while keeping the JES and JER parameters fixed at their central values; we call these the PDF ensembles. In the second set of ensembles, the JES and JER parameters are varied simultaneously, while keeping the PDF parameters fixed to their central values and the renormalization and factorization scales at their nominal values; we call these the JES/JER ensembles.

B.1.1 Generating the PDF ensembles

In the PDF ensembles, each of the six model spectra is sampled from a multivariate Gaussian distribution using the associated 20×20 covariance matrix. For each model spectrum, the covariance matrix is approximated by

$$C_{nm} = \sum_{i=1}^{22} \sum_{j=1}^{22} \Delta X_{ni} \Delta X_{mj}, \quad (6)$$

where $\Delta X_{ni} = (X_{ni}^+ - X_{ni}^-)/2$ and X_{ni}^\pm are the cross section values for n th jet bin associated with the + and - variations of the i th pair of CTEQ6.6 PDF sets. CTEQ [19] publishes approximate 90% intervals. We therefore approximate 68% intervals by dividing each ΔX by 1.64. The correlation induced by the PDF uncertainties across all six model spectra is maintained by using the same set of underlying Gaussian variates during the sampling of the spectra.

B.1.2 Generating the JES/JER ensembles

In the JES/JER ensembles, the JES and JER parameters are sampled simultaneously for the five model spectra QCD_{LO} , and $(\text{QCD} + \text{CI})_{\text{LO}}$ with $\Lambda = 3, 5, 8,$ and 12 TeV, yielding ensembles of correlated shifts from the central JES, JER, and PDF values of the QCD_{LO} and $(\text{QCD} + \text{CI})_{\text{LO}}$ spectra. For example, we compute the spectral residuals $\delta\sigma = \text{QCD}' - \text{QCD}_{\text{central}}$, where QCD' is the shifted jet p_T spectrum and $\text{QCD}_{\text{central}}$ is the jet p_T spectrum computed using the central values of the JES, JER, and PDF parameters. Coherent shifts of the jet energy scale are calculated

for every jet in every simulated event. The jet p_T is shifted by $x\delta$ for each component of the jet energy scale uncertainty, of which there are sixteen, where x is a Gaussian variate of zero mean and unit variance, and δ is a jet-dependent uncertainty for a given component. The contributions from all uncertainty components are summed to obtain an overall shift in the jet p_T . From studies of dijet asymmetry and photon+jet p_T balancing, the uncertainty in the jet energy resolution is estimated to be 10% in the pseudorapidity range $|\eta| < 0.5$ [30]. We sample the jet energy resolution using a procedure identical to that used to sample the jet energy scale, but using a single Gaussian variate.

B.1.3 Generating the JES/JER/PDF ensemble

Another ensemble is created, from the PDF ensembles and the JES/JER ensembles, that approximates simultaneous sampling from the JES, JER, PDF, renormalization, and factorization parameters. We pick at random a correlated set of six spectra from the PDF ensembles, and a correlated set of five spectral residuals from the JES/JER ensembles. The JES/JER spectral residuals $\delta\sigma$ are added to the corresponding shifted spectrum from the PDF ensembles, thereby creating a spectrum in which the JES, JER, PDF, μ_r , and μ_f parameters have been randomly shifted. The NLO QCD spectrum (from the PDF ensembles) is shifted using the LO QCD JES/JER spectral residuals in order to approximate the effect of the JES and JER uncertainties in this spectrum.

The result of the above procedure is an ensemble of sets of properly correlated spectra $\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)$ with $\Lambda = 3, 5, 8$, and 12 TeV, in which the JES, JER, PDF, μ_r and μ_f parameters vary randomly. The ansatz in Eq. (4) is then fitted to the quartet of ratios $[\text{QCD}_{\text{NLO}} + \text{CI}(\Lambda)] / \text{QCD}_{\text{NLO}}$ as described in Section 5.1 to obtain parameter values for p_1, p_2, p_3 , and p_4 . Five hundred sets of these parameters are generated, constituting a discrete approximation to the prior $\pi(\omega) \equiv \pi(p_1, p_2, p_3, p_4)$.

B.2 CL_s calculation

Since CL_s is a criterion rather than a method, it is necessary to document exactly how a CL_s limit is calculated. Such a calculation requires two elements: a test statistic Q that depends on the quantity of interest and its sampling distribution for two different hypotheses, here $\lambda > 0$, which we denote by H_λ , and $\lambda = 0$, which we denote by H_0 . H_λ is the signal plus background hypothesis while H_0 is the background-only hypothesis. For this study, we use the statistic

$$Q(\lambda) = t(D, \lambda) \equiv -2 \ln [p(D|\lambda)/p(D|0)], \quad (7)$$

where $p(D|\lambda)$ is the marginal likelihood

$$\begin{aligned} p(D|\lambda) &= \int p(D|\lambda, \omega) \pi(\omega) d\omega, \\ &\approx \frac{1}{M} \sum_{m=1}^M p(D|\lambda, \omega_m), \end{aligned} \quad (8)$$

where $M = 500$ is the number of points $\omega = p_1, p_2, p_3, p_4$ sampled from the nuisance prior $\pi(\omega)$ described in Appendix B.1. We compute the sampling distributions

$$p(Q|H_\lambda) = \int \delta[Q - t(D, \lambda)] p(D|\lambda) dD, \quad (9)$$

and

$$p(Q|H_0) = \int \delta[Q - t(D, \lambda)] p(D|0) dD, \quad (10)$$

pertaining to the hypotheses H_λ and H_0 , respectively, and solve

$$\text{CL}_s \equiv p(\lambda)/p(0) = 0.05, \quad (11)$$

to obtain a 95 % confidence level (CL_s) upper limit on λ , where the p-value $p(\lambda)$ is defined by

$$p(\lambda) = \Pr[Q(\lambda) > Q_0(\lambda)], \quad (12)$$

and Q_0 is the observed value of Q .

In practice, the CL_s limits are approximated as follows:

1. Choose a value of λ , say λ^* , and compute the observed value of Q , $Q_0(\lambda^*)$.
2. Choose at random one of the $M = 500$ sets of nuisance parameters p_1, p_2, p_3 , and p_4 .
3. Generate a spectrum of $K = 20$ counts, D , according to the multinomial distribution, Eq. (5), with $\lambda = \lambda^*$, which corresponds to the hypothesis H_λ . Compute $Q = t(D, \lambda^*)$ and keep track of how often $Q(\lambda^*) > Q_0(\lambda^*)$. Call this count n_λ .
4. Generate another set of 20 counts, D , but with $\lambda = 0$, corresponding to the hypothesis H_0 . Compute $Q = t(D, \lambda^*)$ and keep track of how often $Q(\lambda^*) > Q_0(\lambda^*)$. Call this count n_0 .
5. Repeat 25,000 times steps 2 to 4, compute $\text{CL}_s \approx n_\lambda/n_0$ and report $\lambda = \lambda^*$ as the upper limit on λ at 95% CL if CL_s is sufficiently close to 0.05; otherwise, keep repeating steps 1 to 4 with different values of λ . The algorithm starts with two values of λ that are likely to bracket the solution and the solution is found using a binary search, which typically requires about 10 to 15 iterations.

B.3 Bayesian calculation

The Bayesian limit calculations use the marginal likelihood, Eq. (8), and two different (formal) priors $\pi(\lambda)$: a prior flat in λ and a reference prior [33–35], which we calculate numerically [35]. An upper limit on λ , λ^* , is computed by solving

$$\int_0^{\lambda^*} p(D|\lambda) \pi(\lambda) d\lambda / p(D) = 0.95, \quad (13)$$

where $p(D)$ is a normalization constant. The integrals are performed using numerical quadrature.

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