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

S. Chatrchyan et al.*
(CMS Collaboration)

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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 $\Lambda$ 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 CLs criterion, lower limits are set on $\Lambda$ 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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I. 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 $\Lambda$. 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 $\Lambda$ 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 (C.L.), for models with destructively and constructively interfering amplitudes, respectively.

The inclusive jet $p_T$ spectrum, i.e., the spectrum of jets in $p + p \rightarrow$ 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).

II. THEORETICAL MODELS

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

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

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

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

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 $\sigma_k$ in the $k$th jet $p_T$ bin is given by

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

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

We use models characterized by the cross section $QCD_{NLO} + CI(\Lambda)$, where $QCD_{NLO} = c_k$ is the inclusive jet cross section computed at next-to-leading order, and $CI(\Lambda) = b_k \lambda + a_k \lambda^2$ parametrizes 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
in the calorimeter resolution function, modified to account for 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 I.

The signal term CI(Λ) is modeled by subtracting the leading-order (LO) QCD jet cross section (QCDLO) 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 QCDNLO. The generated events are processed with the full CMS detector fastNLO program with scenario table fnl232y0.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) $\sigma_{p_T}$ for low-rapidity jets is given by

$$\sigma_{p_T} = p_T \sqrt{\frac{n^2}{p_T^2} + \frac{m^2}{p_T} + c^2},$$

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 cross section ratios, $f = [\text{QCDNLO} + \text{CI}(\Lambda)] / \text{QCDNLO}$, 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 I.

Table I. 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.

<table>
<thead>
<tr>
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<td>1.7 × 10^{-2}</td>
<td>-2.0 × 10^{-5}</td>
<td>4.1 × 10^{-3}</td>
</tr>
</tbody>
</table>

FIG. 1 (color online). The cross section ratios, $f = [\text{QCDNLO} + \text{CI}(\Lambda)] / \text{QCDNLO}$, 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.

FIG. 2 (color online). The cross section ratios, $f = [\text{QCDNLO} + \text{CI}(\Lambda)] / \text{QCDNLO}$, with $\Lambda = 8, 10, 12, \text{and} 14 \text{ TeV}$, for models with destructive (top) and constructive (bottom) interference.
Several functional forms were investigated that gave satisfactory fits, including the ansatz [23]

\[
f = 1 + p_1 \left( \frac{p_T}{100 \text{ GeV}} \right)^{p_2} \left( \frac{\Lambda}{1 \text{ TeV}^{-2}} \right)^{p_3}.
\]

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 Fig. 1. The fit shown in Fig. 1 uses the central values of the JES, JER, and PDF parameters and the renormalization ($\mu_r$) and factorization ($\mu_f$) scales set to $\mu_r = \mu_f = \mu_{QCD}$. Models with constructive interference are obtained by reversing the sign of the parameter $p_1$. The fit parameters are given in Table I. Figures 2 and 3 show model spectra in the jet $p_T$ range $500 \leq p_T \leq 2000$ GeV for values of $\Lambda$ 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 $\Lambda = 10$ TeV, the QCD$_{NLO}$ + CI cross section is lower than the QCD$_{NLO}$ cross section for jet $p_T < 1.3$ TeV. Figure 3 shows the contact interaction signal, CI($\Lambda$), as a function of jet $p_T$.

### III. 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 $\phi$ to be the azimuthal angle, $\theta$ to be the polar angle, and the pseudorapidity to be $\eta = -\ln(\tan(\theta/2))$. 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 $\eta$, using a $p_T$-balancing technique [9], and applied to all components of the jet four momentum.

The results reported are based on data collected using unprescaled 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, ~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 $\sigma_{p_T}$ given in Eq. (3). No jets are observed above 2000 GeV transverse energy.

IV. RESULTS

In Fig. 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 $4.007 \pm 0.009$(stat) fb$^{-1}$ (Sec. V). 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 $Pr(KS) = 0.66$ and the $\chi^2$ per number of degrees of freedom of 23.5/19. Table II 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 $\Lambda$, for models with destructive interference. Figure 6 compares the data with models with constructive interference.

V. 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 $\Lambda$ using the models described in Sec. II. The dominant sources of systematic uncertainties are associated with the JES, the PDFs, the JER, the renormalization ($\mu_r$) and factorization ($\mu_f$) scales, and the modeling parameters of Eq. (4). Nonperturbative corrections are less than 1% for transverse momenta above ~400 GeV [30], negligible compared with other uncertainties, and are therefore not applied to our analysis.

In the search region, the inclusive jet spectrum has a range of 5 orders of magnitude, which causes the limits on $\Lambda$ 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, $N_j$, $j = 1, \ldots, K$, given the observation of a total count $N = \sum_{j=1}^{K} N_j$. The likelihood is then defined by

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

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, $D = N_1, \ldots, N_K$, $\sigma = \sum_{j=1}^{K} \sigma_j$ and $N$ are the total cross section and total observed count, respectively, in the search region, and the symbol $\omega$ denotes the nuisance parameters $p_1, \ldots, p_4$ in Eq. (4).

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, $\omega$, using a discrete representation of the prior $\pi(\omega)$ constructed as described in Sec. VA. This calculation yields the marginal likelihood $p(D|\lambda) = \frac{1}{\pi} \sum_{m=1}^{M} p(D|\lambda, \omega_m)$, 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 Fig. 7.

FIG. 5 (color online). The data compared with model spectra for different values of $\Lambda$ for models with destructive interference (top). The ratio of these spectra to the NLO QCD jet $p_T$ spectrum (bottom).

FIG. 6 (color online). The data compared with model spectra for different values of $\Lambda$ for models with constructive interference (top). The ratio of these spectra to the NLO QCD jet $p_T$ spectrum (bottom).
approximately 20 Gaussian approximation to be valid, we can construct ensembles of six correlated spectra: from the 44 PDF sets. Using these matrices, we generate nuisance parameters. The solid curve is the likelihood marginalizing statistical uncertainties only and the central values of all interference. The dashed curve is the likelihood function including all uncertainties. We have verified that our conclusions are robust with respect to variations in the size of the sample that represents the nuisance prior that incorporates all uncertainties. We use the $\text{CL}_s$ criterion [31,32] to compute upper limits on $\lambda$. For completeness, we give the details of these calculations in Appendix B. Using the procedure described in the Appendix, we obtain 95% lower limits on $\lambda$ 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].

VI. SUMMARY

The inclusive jet $p_T$ spectrum of 7 TeV proton-proton collision events in the ranges $507 \leq p_T \leq 2116$ 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 $\Lambda$ is above 9.9 TeV and 14.3 TeV, respectively, at 95% C.L.

We plan to extend this study to the full 8 TeV CMS data set, making use of a recently released program [36] to calculate

B. Lower limits on $\lambda$

We use the $\text{CL}_s$ criterion [31,32] to compute upper limits on $\lambda$. For completeness, we give the details of these calculations in Appendix B. Using the procedure described in the Appendix, we obtain 95% lower limits on $\lambda$ 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 $9.5 \pm 0.6$ TeV and $13.6 \pm 1.6$ 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 $\lambda$: a prior flat in $\lambda$ and a reference prior [33–35]. Using a flat prior, we find lower limits on $\lambda$ of 10.6 TeV and 14.6 TeV at 95% C.L. 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% C.L., respectively.
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 published to date, have been obtained repriming the classic method to search for contact interactions, namely, searching for deviations from QCD at high jet transverse momentum.

**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 centers 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, operation and maintenance of the LHC and the CMS detector provided by the following funding agencies: BMWF and FWF (Austria); FNRS and FWO (Belgium); CNPq, CAPES, FAPERJ, and FAPESP (Brazil); MEYS (Bulgaria); CERN; CAS, MoST, and NSFC (China); COLCIENCIAS (Colombia); MSES (Croatia); RPF (Cyprus); MoER, SF0690030s09 and ERDF (Estonia); Academy of Finland, MEC, and HIP (Finland); CEA and CNRS/INS2P3 (France); BMBF, DFG, and HGF (Germany); OTKA and NKTH (Hungary); DAE and DST (India); IPM (Iran); SFI (Ireland); INFN (Italy); NRF and WCU (Korea); LAS (Lithuania); CINVESTAV, CONACYT, SEP, and UASLP-FAI (Mexico); MSI (New Zealand); PAEC (Pakistan); MSHE and NSC (Poland); FCT (Portugal); JINR (Armenia, Belarus, Georgia, Ukraine, Uzbekistan); MON, RosAtom, RAS and RFBR (Russia); MSTD (Serbia); SEIDI and CPAN (Spain); Swiss Funding Agencies (Switzerland); NSC (Taipei); ThEPCenter, IPST, and NECTEC (Thailand); TUBITAK and TAEK (Turkey); NASU (Ukraine); STFC (United Kingdom); DOE and NSF (USA).

**APPENDIX A: PYTHIA 6.422 CONTACT INTERACTION CONFIGURATION**

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

**APPENDIX B: STATISTICAL DETAILS**

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$_{\text{NLO}}$, QCD$_{\text{LO}}$, and [QCD + 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 $\mu_r$ and $\mu_F$ 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.

**A. Generating the PDF ensembles**

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

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

where $\Delta X_{ni} = (X_{ni}^+ - X_{ni}^-)/2$ and $X_{ni}^\pm$ are the cross section values for the nth jet bin associated with the + and − variations of the ith pair of CTEQ6.6 PDF sets. CTEQ [19] publishes approximate 90% intervals. We therefore approximate 68% intervals by dividing each $\Delta X$ 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. Generating the JES/JER ensembles**

In the JES/JER ensembles, the JES and JER parameters are sampled simultaneously for the five model spectra QCD$_{\text{NLO}}$, and QCD + CI($\Lambda$)$_{\text{LO}}$ with $\Lambda = 3$, 5, 8, and 12 TeV, yielding ensembles of correlated shifts from the central JES, JER, and PDF values of the QCD$_{\text{NLO}}$ and QCD + CI($\Lambda$)$_{\text{LO}}$ 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 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

<table>
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<th><strong>PYTHIA 6.422 configuration for $\Lambda = 8$ TeV contact interactions.</strong></th>
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<td>CKN(4) = 230</td>
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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 16, where $x$ is a Gaussian variate of zero mean and unit variance, and $\delta$ 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.

C. 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 $\delta r$ are added to the corresponding shifted spectrum from the PDF ensembles, thereby creating a spectrum in which the JES, JER, PDF, $\mu_r$, and $\mu_t$ 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 $Q_{\text{PDF}}$, $Q_{\text{JES}}$, and $Q_{\text{JER}}$, and $\mu_r$, and $\mu_t$ parameters vary randomly. The ansatz in Eq. (4) is then fitted to the quartet of ratios $[Q_{\text{PDF}}/Q_{\text{JES}}]$, $[Q_{\text{PDF}}/Q_{\text{JER}}]$, $[Q_{\text{PDF}}/Q_{\text{PDF}}]$, and $[Q_{\text{PDF}}/Q_{\text{PDF}}]$. Five hundred sets of these parameters are generated, constituting a discrete approximation to the prior $\pi(\omega) \equiv \pi(p_1, p_2, p_3, p_4)$.

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 $H_\lambda$, and $\lambda = 0$, which we denote by $H_0$. $H_\lambda$ is the signal plus background hypothesis while $H_0$ is the background-only hypothesis. For this study, we use the statistic

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

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

$$p(D|\lambda) = \int p(D|\omega) \pi(\omega) d\omega = \frac{1}{M} \sum_{m=1}^{M} p(D|\lambda, \omega_m),$$

(B3)

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 B1. We compute the sampling distributions

$$p(Q|H_\lambda) = \int \delta(Q - t(D, \lambda))p(D|\lambda)dD, \quad (B4)$$

and

$$p(Q|H_0) = \int \delta(Q - t(D, \lambda))p(D|0)dD, \quad (B5)$$

pertaining to the hypotheses $H_\lambda$ and $H_0$, respectively, and solve

$$\text{CL}_s \equiv p(\lambda)/p(0) = 0.05, \quad (B6)$$

and $Q_0$ is the observed value of $Q$.

In practice, the CL$_s$ limits are approximated as follows:

1. Choose a value of $\lambda$, say $\lambda^*$, and compute the observed value of $Q$, $Q_0(\lambda^*)$.
2. Choose at random one of the $M = 500$ sets of nuisance parameters $p_1, p_2, p_3, p_4$.
3. Generate a spectrum of $K = 20$ counts, $D$, according to the multinomial distribution, Eq. (5), with $\lambda = \lambda^*$, which corresponds to the hypothesis $H_\lambda$. Compute $Q = t(D, \lambda^*)$ and keep track of how often $Q(\lambda^*) > Q_0(\lambda^*)$. Call this count $n_1$.
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 $\text{CL}_s \approx n_1/n_0$, and report $\lambda = \lambda^*$ as the upper limit on $\lambda$ at 95% C.L. if $\text{CL}_s$ is sufficiently close to 0.05; otherwise, keep repeating steps 1 to 4 with different values of $\lambda$. The algorithm starts with two values of $\lambda$ that are likely to bracket the solution and the solution is found using a binary search, which typically requires about 10–15 iterations.

3. Bayesian calculation

The Bayesian limit calculations use the marginal likelihood, Eq. (B3), and two different (formal) priors $\pi(\lambda)$: a prior flat in $\lambda$ and a reference prior [33–35], which we calculate numerically [35]. An upper limit on $\lambda$, $\lambda^*$ is computed by solving

$$\int_0^{\lambda^*} p(D|\lambda)\pi(\lambda)d\lambda/p(D) = 0.95, \quad (B8)$$

where $p(D)$ is a normalization constant. The integrals are performed using numerical quadrature.
SEARCH FOR CONTACT INTERACTIONS USING THE ...
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125 Cornell University, Ithaca, New York, USA
126 Fairfield University, Fairfield, Connecticut, USA
127 Fermi National Accelerator Laboratory, Batavia, Illinois, USA
128 University of Florida, Gainesville, Florida, USA
129 Florida International University, Miami, Florida, USA
130 Florida State University, Tallahassee, Florida, USA
131 Florida Institute of Technology, Melbourne, Florida, USA
132 University of Illinois at Chicago (UIC), Chicago, Illinois, USA
133 The University of Iowa, Iowa City, Iowa, USA
134 Johns Hopkins University, Baltimore, Maryland, USA
135 The University of Kansas, Lawrence, Kansas, USA
136 Kansas State University, Manhattan, Kansas, USA
137 Lawrence Livermore National Laboratory, Livermore, California, USA
138 University of Maryland, College Park, Maryland, USA
139 Massachusetts Institute of Technology, Cambridge, Massachusetts, USA
140 University of Minnesota, Minneapolis, Minnesota, USA
141 University of Mississippi, Oxford, Mississippi, USA
142 University of Nebraska-Lincoln, Lincoln, Nebraska, USA
143 State University of New York at Buffalo, Buffalo, New York, USA
144 Northeastern University, Boston, Massachusetts, USA
145 Northwestern University, Evanston, Illinois, USA
146 University of Notre Dame, Notre Dame, Indiana, USA
147 The Ohio State University, Columbus, Ohio, USA
148 Princeton University, Princeton, New Jersey, USA
149 University of Puerto Rico, Mayaguez, Puerto Rico
150 Purdue University, West Lafayette, Indiana, USA
151 Purdue University Calumet, Hammond, Indiana, USA
152 Rice University, Houston, Texas, USA
153 University of Rochester, Rochester, New York, USA
154 The Rockefeller University, New York, New York, USA
155 Rutgers, The State University of New Jersey, Piscataway, New Jersey, USA
156 University of Tennessee, Knoxville, Tennessee, USA
157 Texas A&M University, College Station, Texas, USA
158 Texas Tech University, Lubbock, Texas, USA
159 Vanderbilt University, Nashville, Tennessee, USA
160 University of Virginia, Charlottesville, Virginia, USA
161 Wayne State University, Detroit, Michigan, USA
162 University of Wisconsin, Madison, Wisconsin, USA

a Deceased.
b Also at Vienna University of Technology, Vienna, Austria.
c Also at CERN, European Organization for Nuclear Research, Geneva, Switzerland.
d Also at National Institute of Chemical Physics and Biophysics, Tallinn, Estonia.
e Also at California Institute of Technology, Pasadena, CA, USA.
f Also at Laboratoire Leprince-Ringuet, Ecole Polytechnique, IN2P3-CNRS, Palaiseau, France.
g Also at Suez Canal University, Suez, Egypt.
h Also at Zewail City of Science and Technology, Zewail, Egypt.
i Also at Cairo University, Cairo, Egypt.
j Also at Fayoum University, El-Fayoum, Egypt.
k Also at Helwan University, Cairo, Egypt.
l Also at British University in Egypt, Cairo, Egypt.
m Now at Ain Shams University, Cairo, Egypt.
n Also at National Centre for Nuclear Research, Swierk, Poland.
o Also at Université de Haute Alsace, Mulhouse, France.
p Also at Joint Institute for Nuclear Research, Dubna, Russia.
q Also at Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow, Russia.
r Also at Brandenburg University of Technology, Cottbus, Germany.
s Also at The University of Kansas, Lawrence, KS, USA.
t Also at Institute of Nuclear Research ATOMKI, Debrecen, Hungary.
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u Also at Eötvös Loránd University, Budapest, Hungary.

v Also at Tata Institute of Fundamental Research - HECR, Mumbai, India.

w Now at King Abdulaziz University, Jeddah, Saudi Arabia.

x Also at University of Visva-Bharati, Santiniketan, India.

y Also at Sharif University of Technology, Tehran, Iran.

z Also at Isfahan University of Technology, Isfahan, Iran.

aa Also at Shiraz University, Shiraz, Iran.

bb Also at Plasma Physics Research Center, Science and Research Branch, Islamic Azad University, Tehran, Iran.

cc Also at Facoltà Ingegneria, Università di Roma, Roma, Italy.

dd Also at Università degli Studi Guglielmo Marconi, Roma, Italy.

ee Also at Università degli Studi di Siena, Siena, Italy.

ff Also at University of Bucharest, Faculty of Physics, Bucuresti-Magurele, Romania.

gg Also at Faculty of Physics of University of Belgrade, Belgrade, Serbia.

hh Also at University of California, Los Angeles, CA, USA.

ii Also at Scuola Normale e Sezione dell’INFN, Pisa, Italy.

jj Also at INFN Sezione di Roma, Roma, Italy.

kk Also at University of Athens, Athens, Greece.

ll Also at Rutherford Appleton Laboratory, Didcot, United Kingdom.

mm Also at Paul Scherrer Institut, Villigen, Switzerland.

nn Also at Institute for Theoretical and Experimental Physics, Moscow, Russia.

oo Also at Albert Einstein Center for Fundamental Physics, Bern, Switzerland.

pp Also at Gaziosmanpasa University, Tokat, Turkey.

qq Also at Adiyaman University, Adiyaman, Turkey.

rr Also at Izmir Institute of Technology, Izmir, Turkey.

ss Also at The University of Iowa, Iowa City, IA, USA.

tt Also at Mersin University, Mersin, Turkey.

uu Also at Ozyegin University, Istanbul, Turkey.

vv Also at Kafkas University, Kars, Turkey.

ww Also at Suleyman Demirel University, Isparta, Turkey.

xx Also at Ege University, Izmir, Turkey.

yy Also at School of Physics and Astronomy, University of Southampton, Southampton, United Kingdom.

zz Also at INFN Sezione di Perugia, Università di Perugia, Perugia, Italy.

aaa Also at Utah Valley University, Orem, UT, USA.

bbb Now at University of Edinburgh, Scotland, Edinburgh, United Kingdom.

ccc Also at Institute for Nuclear Research, Moscow, Russia.

ddd Also at University of Belgrade, Faculty of Physics and Vinca Institute of Nuclear Sciences, Belgrade, Serbia.

eee Also at Argonne National Laboratory, Argonne, IL, USA.

fff Also at Erzincan University, Erzincan, Turkey.

ggg Also at Mimar Sinan University, Istanbul, Istanbul, Turkey.

hhh Also at KFKI Research Institute for Particle and Nuclear Physics, Budapest, Hungary.

iii Also at Kyungpook National University, Daegu, Korea.