Editors' Suggestion

Measurement of Energy Correlators inside Jets and Determination of the Strong Coupling $\alpha_S(m_Z)$

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Energy correlators that describe energy-weighted distances between two or three particles in a hadronic jet are measured using an event sample of $\sqrt{s} = 13$ TeV proton-proton collisions collected by the CMS experiment and corresponding to an integrated luminosity of 36.3 fb^{-1}. The measured distributions are consistent with the trends in the simulation that reveal two key features of the strong interaction: confinement and asymptotic freedom. By comparing the ratio of the measured three- and two-particle energy correlator distributions with theoretical calculations that resum collinear emissions at approximate next-to-next-to-leading-logarithmic accuracy matched to a next-to-leading-order calculation, the strong coupling is determined at the Z boson mass: $\alpha_S(m_Z) = 0.1229^{+0.0040}_{-0.0050}$, the most precise $\alpha_S(m_Z)$ value obtained using jet substructure observables.

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In high-energy proton-proton (pp) collisions, quarks and gluons undergo cascades of radiation and hadronization processes, resulting in the production of hadrons that can cluster in jets. Collisions at the LHC have produced an unprecedented number of events containing jets, spanning a broad range of energies. Studies of jets provide information on the strong interaction, described by quantum chromodynamics (QCD) [1]. Jet substructure has been widely studied at the LHC [2–11]. Comparing high-precision measurements of jet substructure observables with Monte Carlo (MC) simulations and perturbative QCD (pQCD) calculations improves our understanding of QCD.

New observables have been recently proposed to describe multiparticle energy correlations within jets [12]. They evolved from the event shape observable energy-energy correlator (EEC) [13], which was extensively studied in e^+e^- experiments [14–17]. The new observables study correlations inside jets, therefore being more sensitive than EEC in the small angle limit [18]. They are derived from energy-flow operators, are collinear- and infrared-safe [19], and can be formulated with correlation functions of light-ray operators [20–23] widely used in conformal field theory. Analytical calculations with all-orders resummation at next-to-leading-logarithmic (NLL) [24,25] and approximate next-to-NLL ($\mathrm{NNLL_{approx}}$) [26] accuracy in pQCD, matched to next-to-leading-order (NLO) pQCD calculations, denoted as $\mathrm{NLO + NNLL_{approx}}$, can be achieved for these observables. This allows comparisons between theory and data with 5% accuracy [26]. We focus on the two- and three-particle energy correlators (E2C and E3C, respectively), for which there are predictions with $\mathrm{NLO + NNLL_{approx}}$ precision [26].

Studies of jet substructure can be used to determine the strong coupling α_S [27–30]. Among the interaction couplings of the standard model, α_S is the least precisely known [31]. The world average α_S at the Z boson mass is $\alpha_S(m_Z) = 0.1180$, with a 0.8% precision [31]. Methods that mainly rely on fixed-order calculations provide α_S extractions with 1%–3% precision at the LHC [32–37]; jet substructure is more sensitive to collinear physics effects, allowing for measurements in complementary phase space regions. In these regions, studies based on event shapes in e^+e^- collisions at LEP [38–40] obtained a value of α_S about 5% lower than the world average, emphasizing the importance of new studies. It has been estimated that a value of α_S with 10% precision could be achieved using the soft-drop groomed jet mass [27]. There are two major difficulties in reaching a high-precision α_S extraction with this observable: its dependence on the relative fraction of quark- and gluon-initiated jets, since a larger gluon jet fraction can be misinterpreted as a larger α_S value; and the large uncertainty in the nonperturbative corrections. A jet substructure measurement using heavy-flavor jets provided an α_S value with ≈10% precision [41]. Other approaches have been proposed to tackle the parton-flavor dependence [30]. An approach based on the ratio of multiparticle energy correlators was proposed to solve both problems and improve the precision of jet substructure α_S determinations [12].

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Unlike observables such as the jet charge, which provide a single value for each jet, E2C and E3C provide distributions, because each jet has many particles and, hence, many pairs and triplets. These distributions depend on x_L, defined as the angular distance between the two particles of the E2C pair, $\sqrt{(\Delta\eta_{i,j})^2 + (\Delta\phi_{i,j})^2}$, where $\Delta\eta$ and $\Delta\phi$ are the distances in pseudorapidity and azimuthal angle of the particles, respectively, or as the largest angular distance among the three pair combinations of an E3C triplet. A jet with n particles contributes n^2 entries to the E2C x_L distribution, each having a weight $E_i E_j/E^2$, the product of the fractional energy of the jet carried by each of the particles. The entry with $j = i$ adds to the $x_L = 0$ bin, which contributes to the overall normalization of the distribution. Similarly, a jet contributes n^3 entries to the E3C x_L distribution, with weights $E_i E_j E_k/E^3$, where the indices represent the three particles in the triplet. The fractional energy weights ensure that E2C and E3C are insensitive to soft radiation, without the need for jet grooming techniques [12], and that their distributions are normalized to the number of jets in the event sample. Additionally, taking the ratio of two energy correlators further suppresses nonperturbative effects.

The distinctive shape of the x_L-differential E2C and E3C correlators provides information on the timescale of hadron formation, still an open question in QCD [1]. The different x_L regions probe the dynamics of jet formation, governed by the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi evolution equations [42–45]. Most jet substructure observables are dominated by terms proportional to the coupling α_S, to a large logarithm due to collinear divergences $\ln x_L$, and to a color factor C_i [27]. The quark-gluon composition, essential to extract α_S, can be calculated from parton distribution functions (PDFs), at the price of introducing large uncertainties [27]. The PDF dependence is largely suppressed in the E3C/E2C ratio, which remains sensitive to α_S because E3C and E2C have different dependences on α_S, C_i, and its higher-order expansion terms. The calculation at leading-logarithmic accuracy implies that the ratio is approximately linear in $\alpha_S \ln x_L$ [12], so that measuring its slope with respect to $\ln x_L$, as a function of the jet momentum transverse to the pp collision axis (p_T), gives the dependence of α_S on the jet energy.

In this Letter, we report the E2C and E3C distributions versus x_L and the $\alpha_S(m_Z)$ value obtained by comparing their ratio with theoretical predictions at NLO + $\mathrm{NNLL_{approx}}$ accuracy [26]. This is the first measurement of E2C at a hadron collider, probing a much higher energy scale than at the e^+e^- experiments, and the first ever measurement of E3C. The analysis is based on an event sample of pp collisions at $\sqrt{s} = 13$ TeV collected by CMS in 2016 and corresponding to an integrated luminosity of 36.3 fb^{-1} [46]. The CMS detector has been designed [47] to trigger on [48,49] and identify electrons, muons, photons, and hadrons [50–53]. The particles are reconstructed [54–56] from information provided by a silicon tracker, an electromagnetic calorimeter, and a hadron calorimeter, placed in a 3.8 T superconducting solenoid, and by muon detectors placed outside.

The hadronic jets are clustered with the anti-k_T algorithm [57,58] with a resolution parameter of 0.4, a value suited for parton shower (PS) studies at relatively small angles [25,26]. The jet four-momentum is determined as the vectorial sum of all particle four-momenta in the jet. We select the dijet process to measure E2C and E3C because of its large cross section and wide energy range. Background processes beyond those produced by the strong interaction have a negligible contribution [33], allowing for a direct comparison between data and predictions. A series of eight triggers are used, each requiring a leading jet with increasing p_T thresholds, the lowest one being 60 GeV. The events must contain at least two jets, with $p_T > 97$ GeV and $|\eta| < 2.1$. The η selection ensures that the jet constituents are reconstructed with good spatial and momentum resolutions. In addition, the two leading jets are required to be back to back in the transverse plane, with $|\Delta\phi| > 2$. Jets with lower p_T are not considered, because the corresponding pQCD calculations can be performed only in a limited x_L range, so that the different stages in jet formation cannot be reliably identified. To study the E2C and E3C energy dependence, the two leading jets in each event are binned in eight p_T bins, in the 97–1784 GeV range. The boundaries are optimized so that the corresponding trigger has an efficiency exceeding 99.5% [33]. Weights corresponding to the trigger prescales are applied [48]. All the neutral and charged particles with $p_T > 1$ GeV within the jets are used to compute the energy correlators. Each jet contributes multiple entries to the E2C and E3C distributions, and each event provides two leading jets, causing statistical correlations across x_L and p_T bins, amounting to 40% on average. Covariance matrices are calculated for the two distributions. Since the analysis is not statistically limited, we measure the E2C and E3C distributions from two independent data samples, built by splitting the data in two halves, to avoid keeping track of the correlations between the two variables, which would lead to larger matrices and computational challenges.

In order to obtain the E2C and E3C distributions at particle level, we unfold the measured distributions for the detector response, using the iterative D'Agostini unfolding method [59], implemented in RooUnfold [60,61]. We stop the iterations once the p value between consecutive unfolded distributions exceeds 0.05, meaning that the distributions become statistically consistent. The reconstructed jets and particles are considered matched to the generated ones if their relative angular distance is smaller than 0.2 and 0.05, respectively. If multiple matches are found, the one with the closest p_T is chosen. The jet matching efficiency is above 99%. The fractions of correctly matched charged particles, photons, and neutral particles are 80%–84%, 54%–70%, and 20%–35%, respectively, corresponding to 88%–95%, 80%–97%, and 40%–92% of the total energy of these particle types. The unmatched objects are considered to be misreconstructed, and their contribution is subtracted from the data. After unfolding, bin-by-bin inefficiency corrections are applied, derived from the particle-level unmatched objects. Given the correlations between the variables, the unfolding is performed in three dimensions: x_L, p_T, and the energy weight. Simulations are used to derive the response matrices.

Four samples of simulated events are used to model hadronization effects and to evaluate the detector response. They are generated with PYTHIA8.240 [62], HERWIG7.1.4 [63,64], and MadGraph5_aMC@NLO [65,66], the latter being interfaced with PYTHIA8 or HERWIG7. Dijet events are generated at leading order (LO) in pQCD, with NNPDF3.1 PDFs [67], and interfaced with GEANT4 [68]. In the MadGraph5_aMC@NLO samples, final states with up to four partons are generated at tree level, and the MLM jet matching scheme is applied [66]. Simulated pileup interactions are included, normalized to a total inelastic cross section of 69.2 mb [69]. The unfolding uses the PYTHIA8 event sample, which is the largest one. Other event samples are generated at the particle level to provide predictions that can be directly compared with the (unfolded) measured distributions. They reflect several alternative PS and hadronization models. More details of the simulated samples can be found in Supplemental Material [70].

The energy scale uncertainty of the jet constituents, 3% for photons, 5% for neutral particles, and 1% for charged particles, affects the energy of these particles and, hence, the jet p_T. The track reconstruction efficiency uncertainty, 3%, reflects the mismodeling of the efficiency to reconstruct charged-particle tracks in the dense core of the jets [56]. The MC event generators differ in the PS and hadronization modeling, in the tuning of parameters, and in the fixed-order matrix calculation for the hard scattering. These differences are not covered by the renormalization scale uncertainty nor by varying the underlying event (UE) in PYTHIA8. Therefore, we use the differences between the results obtained with the baseline PYTHIA8 MC and the other samples to evaluate one-sided uncertainties in the MC modeling. The (unfolded) particle-level data distributions are recomputed with the responses corresponding to the variations mentioned above, to establish their uncertainty. The variations in MC modeling contribute the largest source of uncertainty, 2%–10% depending on x_L and p_T, followed by the neutral particle energy scale, which contributes an uncertainty of 1%–2%.

The measured (unfolded) E2C distributions are shown in Fig. 1, in four illustrative jet p_T ranges, together with the predictions of three models: PYTHIA8 (with the CP5 tune and p_T-ordered showers), HERWIG7 (with the CH3 tune and angular-ordered showers), and SHERPA2 (with default settings). The E2C distributions in the other four jet p_T ranges, the E3C distributions, and comparisons with all the considered MC models are collected in Supplemental Material [70], while tabulated results are provided in the HEPData record for this analysis [74]. The lower panels show the ratios between the data and the PYTHIA8 reference. The uncertainty in the PYTHIA8 MC prediction (blue band) reflects the following sources. The uncertainties from the missing higher orders in the hard scattering computation and from the PS modeling are obtained by independently varying the renormalization and factorization scales by factors of 0.5 and 2, respectively, keeping their ratio between 0.5 and 2. The PDF uncertainty is evaluated using an envelope of 100 PDF sets, corresponding to the variations of the uncertainty eigenvectors of the default set. The uncertainty in the infrared approximation of the PYTHIA8 PS splitting kernels is evaluated by varying the coefficient of the nonsingular term by ±2 [75]. The

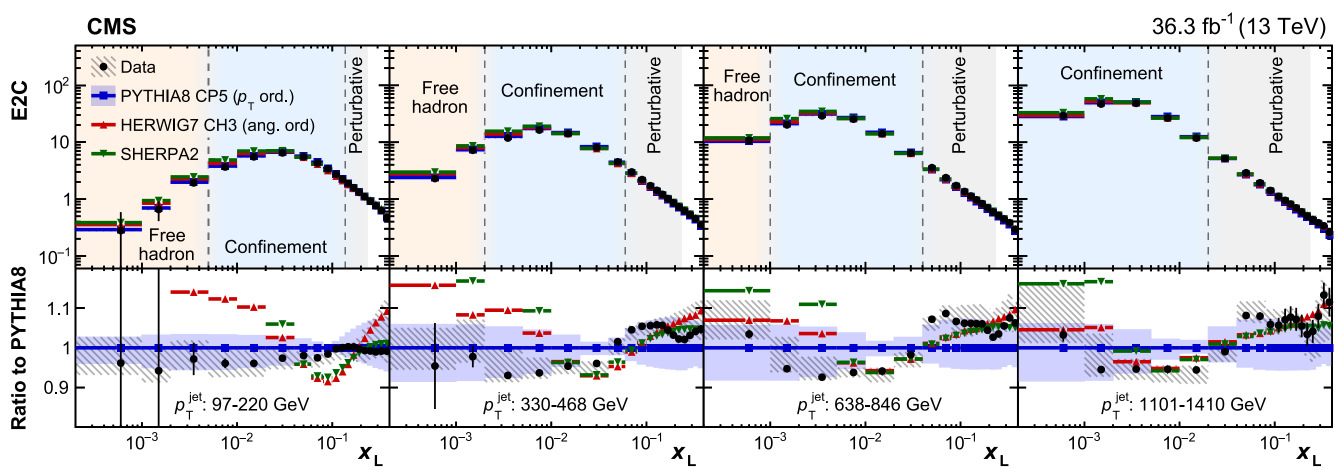

FIG. 1. Measured (unfolded) and simulated E2C x_L distributions, in four p_T bins. The lower panels show the ratios to the PYTHIA8 reference. The data statistical (bars) and systematic (boxes) uncertainties are also shown, as is the PYTHIA8 uncertainty (blue band).

uncertainty in the UE model is evaluated by using the Monash tune [76]. The measured and PYTHIA8 distributions show good agreement, given the uncertainties. The lower panels in Fig. 1 also show the ratios between the HERWIG7 and SHERPA2 MC distributions and the PYTHIA8 reference, to illustrate the level of variation that exists among models.

Since the MC models provide a reasonably good description of the measured x_L dependence of E2C, we can discuss it in terms of three phases in the evolution of the produced jets. The momentum exchange between two particles is proportional to $p_T x_L$ [12], so that x_L reflects the energy scale of the interaction. In the large x_L region, dominated by wide-angle splittings from the emission of additional partons during the PS stage, we see that E2C decreases as x_L increases, as predicted by pQCD [25]. The small x_L region, where we have the opposite trend, reflects a phase dominated by noninteracting hadrons. The intermediate x_L region corresponds to a transition phase, where the partons get confined in the final hadrons. To determine the x_L boundaries, shown as dashed vertical lines in Fig. 1, we fit the x_L distributions in each jet p_T range and identify the regions that follow the quantitative scaling predictions: In the free-hadron region, the E2C and E3C particle-level distributions are expected to increase with x_L as $\exp(2 \ln x_L)$ [77]; in the perturbative region, the E3C/E2C ratio of parton-level distributions is expected to increase with x_L as $\ln x_L$ [26], with small differences at the hadron level. The fits of the parton- and hadron-level distributions are made using the simulated trends, which describe well the shapes of the measured distributions. As the jet p_T increases, the boundaries shift toward smaller x_L, so that the energy scale at which the transition occurs, $Q = a p_T x_L$ [12], remains the same. The constant a is unknown, but the boundaries derived from simulation suggest that $Q/a \approx 20$ GeV for the transition between the perturbative and confinement regions and ≈ 0.8 GeV for the transition between the confinement and free-hadron regions. The boundaries are sensitive to α_S. We compare only data and pQCD where the calculations are reliable.

Figure 2 shows the ratio between the E3C and E2C x_L distributions, both measured and predicted at NLO + NNLL$_{\mathrm{approx}}$ [26]. The renormalization scale is set to $p_T^{\mathrm{jet}} R/2$ in each region, where $R = 0.4$. This choice approximates the energy scale of the parton splitting and improves the convergence of the pQCD calculation [26]. Hadronization and UE effects are corrected using PYTHIA8 and HERWIG7 simulations, accounting for the 1 GeV threshold on the hadron p_T. The corrections are applied to the parton-level calculations and are in the 5%–40% range for the E2C and E3C distributions, decreasing with increasing x_L and jet p_T; they largely cancel in the ratio, decreasing to the 0%–3% range. The difference between the PYTHIA8 and HERWIG7 correction factors is considered as the nonperturbative theoretical uncertainty [33]. Figure 3 shows the slope of the x_L dependence of the E3C over E2C ratio, defined as

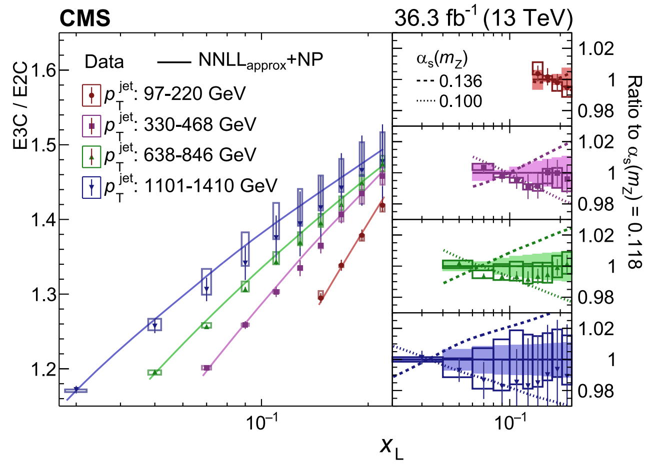

FIG. 2. Measured E3C/E2C ratio (left) and their ratio to predictions (right) in the perturbative x_L region and four jet p_T bins. The NLO + NNLL$_{\mathrm{approx}}$ predictions [26] are corrected to hadron level and normalized to the data. The statistical and experimental systematic uncertainties are shown with bars and boxes, respectively.

$\Delta(\mathrm{E3C/E2C})/\Delta \log x_L$, accounting for the covariance matrix and systematic uncertainties. Since the slope is approximately proportional to $\alpha_S(Q)$ [12], the trend reflects the running of α_S with jet energy.

Comparing the measured E3C/E2C ratio, as a function of x_L, with the corresponding theoretical predictions (using the median value of the predictions in each x_L bin), we obtain χ^2 values as a function of $\alpha_S(m_Z)$. We consider the theoretical uncertainties described above, except that the PS renormalization scale uncertainty is replaced by the NLO + NNLL$_{\mathrm{approx}}$ uncertainty [26]. Only the perturbative region is used; the $x_L < 0.234$ selection avoids boundary effects of

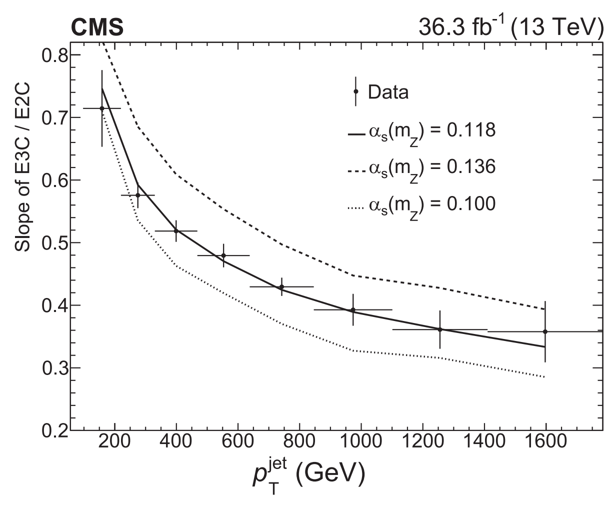

FIG. 3. Fitted slopes of the measured E3C/E2C ratios, in the eight jet p_T bins, compared to theoretical predictions for three α_S values.

the jet clustering algorithm [25]. Since the theory normalization is unknown in the perturbative region, a free parameter is introduced in each p_T bin, and we consider only the shape effects of the uncertainties. For each $\alpha_S(m_Z)$ value, the χ^2 is defined as

$$\chi^2 = [\vec{v}_m(\vec{\theta}) - \vec{v}_{\text{th}}(\alpha_S, \vec{\theta})]^\intercal V_m^{-1} [\vec{v}_m(\vec{\theta}) - \vec{v}_{\text{th}}(\alpha_S, \vec{\theta})] + \sum_j \theta_j^2,$$

where the variables v_m and v_{th} are the measured and predicted differential E3C/E2C ratios, respectively, and V_m is the covariance matrix of the unfolded data. The experimental and theoretical uncertainties are considered through n nuisance parameters, $\vec{\theta} = (\theta_1, \ldots, \theta_n)$, where θ_j is the number of standard deviations by which the uncertainty "j" is varied. The θ_j variation changes the shapes of the E2C and E3C distributions simultaneously across all the bins.

The best-fit value of $\alpha_S(m_Z)$ is $0.1229^{+0.0014}_{-0.0012}(\text{stat})\,^{+0.0030}_{-0.0033}(\text{theo})\,^{+0.0023}_{-0.0036}(\text{exp})$, where theo and exp stand for theoretical and experimental systematic uncertainties, respectively. The central value is determined by minimizing the χ^2 with respect to the nuisance parameters, simultaneously varied, and the uncertainties are given by the $\alpha_S(m_Z)$ values that lead to χ^2 values exceeding the minimum by 1. The high precision stems from the cancelation of most E2C and E3C systematic uncertainties in their ratio. The largest sources of uncertainty are the renormalization scale in the theoretical calculation (2.4%) and the energy scales of the jet constituents (2.3%).

In summary, the two- and three-particle jet substructure observables E2C and E3C have been measured using a sample of proton-proton collision events at $\sqrt{s} = 13$ TeV, collected by the CMS experiment and corresponding to an integrated luminosity of 36.3 fb^{-1}. A multidimensional unfolding has been performed, of the jet p_T, of the (largest) distance between particles in a pair or a triplet, and of the product of their energy weights, to compare the data with distributions simulated with several parton showering and hadronization models. This high-precision measurement of jet properties described by QCD can help validate future higher-order corrections in parton shower algorithms. The strong coupling at the Z boson mass is extracted by comparing the measured E3C/E2C ratio with calculations at approximate next-to-next-to-leading-logarithmic accuracy matched to a next-to-leading perturbative QCD order corrected for nonperturbative effects. The result $\alpha_S(m_Z) = 0.1229^{+0.0040}_{-0.0050}$ is consistent with the world average 0.1180. This is the most precise determination of α_S using jet substructure techniques. The result benefits from the development of novel jet substructure observables, which reduce the sensitivity to the quark-gluon composition, and from the availability of high-precision theoretical calculations.

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