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Measurement of the Soft-Drop Jet Mass in $pp$ Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector

M. Aaboud et al.*
(The ATLAS Collaboration)

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Jet substructure observables have significantly extended the search program for physics beyond the standard model at the Large Hadron Collider. The state-of-the-art tools have been motivated by theoretical calculations, but there has never been a direct comparison between data and calculations of jet substructure observables that are accurate beyond leading-logarithm approximation. Such observables are significant not only for probing the collinear regime of QCD that is largely unexplored at a hadron collider, but also for improving the understanding of jet substructure properties that are used in many studies at the Large Hadron Collider. This Letter documents a measurement of the first jet substructure quantity at a hadron collider to be calculated at next-to-next-to-leading-logarithm accuracy. The normalized, differential cross section is measured as a function of log$_{10}(\rho^2)$, where $\rho$ is the ratio of the soft-drop mass to the ungroomed jet transverse momentum. This quantity is measured in dijet events from 32.9 fb$^{-1}$ of $\sqrt{s} = 13$ TeV proton-proton collisions recorded by the ATLAS detector. The data are unfolded to correct for detector effects and compared to precise QCD calculations and leading-logarithm particle-level Monte Carlo simulations.

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The dynamics of strong interactions, described by quantum chromodynamics (QCD), are responsible for most of the physical processes occurring in proton-proton ($pp$) scattering at the Large Hadron Collider (LHC). The fundamental particles of QCD, quarks and gluons, cannot be observed directly and instead form collimated sprays of particles called jets when produced at high energy. The radiation pattern inside jets has been used extensively for identifying highly Lorentz boosted hadronically decaying massive particles [1]. Many of these techniques were motivated by recent advances in analytical calculations of jet substructure [8]. However, prior to this work, there has never been a direct comparison between collision data and calculations beyond the leading-logarithm (LL) accuracy of parton shower (PS) Monte Carlo (MC) programs [9]. The comparisons presented here begin the field of precision jet substructure, wherein data and calculations in the collinear regime of QCD can be used to test the modeling of final state radiation and maybe even extract fundamental parameters of the SM such as the strong coupling constant or the top quark mass [10]. Such precision understanding will also be essential to maximize the quantitative sensitivity of the LHC and future colliders to physics beyond the standard model.

Of particular importance is the jet mass, defined as the norm of the four-momentum sum of constituents inside a jet. The jet mass is a key jet substructure observable and is the most powerful tool for identifying Lorentz boosted hadronically decaying massive particles. Unlike Lorentz boosted bosons or top quarks, the mass of generic quark and gluon jets is set by the fragmentation of highly virtual partons [11]. A complete prediction for mass or other variables beyond LL has not been possible due to the presence of nonglobal logarithms (NGLs) [12]: resummation terms associated with particles that radiate out of, and then radiate back into, a jet. These terms are formally present at next-to-leading-logarithm (NLL) accuracy and have prevented full comparisons of observables beyond LL. However, using insights from modern analytical methods, the authors of Ref. [13] introduced a new procedure to systematically remove soft and wide-angle radiation from the jet (grooming) that is formally insensitive to NGLs. This procedure was extended in Ref. [14] to form the soft-drop grooming algorithm. The calculation of the masses of jets that have the soft-drop procedure applied is insensitive to NGLs. The distribution of the soft-drop mass has now been calculated at both next-to-leading order (NLO) with NLL [15,16] and leading order (LO) with next-to-next-to-leading-logarithm (NNLL) accuracy [17,18]. These are the most precise calculations for jet substructure at a hadron collider.

The soft-drop procedure acts on the clustering history of a sequential recombination jet algorithm [19]. In these
algorithms, all inputs to jet-finding start as a proto-jet and are combined pairwise using a distance metric in $y$-$\phi$ space [20]. When the smallest distance is above some threshold $R$ (called the jet radius), the algorithm terminates and the remaining proto-jets are the final jets. The clustering history is the sequence of pairwise combinations that lead to a particular jet. Jets at the LHC experiments are usually clustered using the anti-$k_t$ algorithm [21], which has the benefit of producing regularly shaped jets in $y$-$\phi$ space. Even though anti-$k_t$ jets are useful experimentally, their clustering history does not mimic the angular-ordered PS [22] used in the related $k_t$ [19,23] and Cambridge-Aachen [24,25] (C/A) algorithms. The soft-drop algorithm starts by reclustering an anti-$k_t$ jet’s constituents with the C/A algorithm. Next, the clustering tree is traversed from the latest branch to the earliest and at each node the following criterion is applied to proto-jets $j_1$ and $j_2$:

$$\frac{\min(p_{T,j_1}, p_{T,j_2})}{p_{T,j_1} + p_{T,j_2}} > z_{\text{cut}} \left( \frac{\Delta R_{12}}{R} \right)^\beta,$$  

(1)

where $p_T$ is the momentum of a jet transverse to the beam pipe, $z_{\text{cut}}$ and $\beta$ are algorithm parameters, and $\Delta R_{12} = \sqrt{(\Delta y)^2 + (\Delta \phi)^2}$ is the distance in $y$-$\phi$ between the proto-jets. The parameter $z_{\text{cut}}$ sets the scale of the energy removed by the algorithm; $\beta$ tunes the sensitivity of the algorithm to wide-angle radiation. If the soft-drop condition in Eq. (1) is not satisfied, then the branch with the smaller $p_T$ is removed. The procedure is then iterated on the remaining branch. If the condition is satisfied at any node, the algorithm terminates. As $\beta$ increases, the fraction of branches where the condition is satisfied increases, reducing the amount of radiation removed from the jet. In the limit $\beta \rightarrow \infty$, the original jet is untouched. The mass of the resulting jet is referred to as the soft-drop jet mass, $m_{\text{soft drop}}$.

This Letter presents a measurement of the soft-drop jet mass using 32.9 fb$^{-1}$ of $\sqrt{s} = 13$ TeV $p$-$p$ data collected in 2016 by the ATLAS detector, and the first comparison to predictions of jet substructure that are formally more accurate than the LL PS approximation.

ATLAS is a particle detector designed to achieve nearly a 4$\pi$ coverage in solid angle [26]. The inner tracking detector (ID) is inside a 2 T magnetic field and is designed to measure charged-particle trajectories up to $|\eta| = 2.5$. Surrounding the ID are electromagnetic and hadronic calorimeters, which use liquid argon and lead, copper, or tungsten absorber for the electromagnetic and forward ($|\eta| > 1.7$) hadronic detectors, and scintillator-tile active material with steel absorber for the central ($|\eta| < 1.7$) hadronic calorimeter.

For this study, jets are clustered using the anti-$k_t$ jet algorithm with radius parameter $R = 0.8$ implemented in FASTJET [27]. The inputs are topological calorimeter-cell clusters calibrated using the local cluster weighting algorithm [28]. In order to improve the rapidity resolution, cluster four-vectors are corrected to point toward the reconstructed primary collision vertex [29].

An overall jet energy calibration, derived for $R = 0.8$ jets, accounts for residual detector effects as well as contributions from pileup (i.e., simultaneous additional $p$-$p$ collisions) in order to make the reconstructed jet energy unbiased (up through “absolute MC-based calibration” in Ref. [30]). Jets are required to have $|\eta| < 1.5$ so that their calorimeter-cell clusters are within the coverage of the ID.

Events were selected online using a two-level trigger system [31] that is hardware-based at the first level and software-based for the second level. In this analysis, the full-luminosity jet trigger with the lowest $p_T$ threshold is nearly 100% efficient for jets with $p_T > 600$ GeV. Events are required to have a minimum of two jets, at least one of which has $p_T > 600$ GeV. In addition, a dijet topology is imposed by requiring that the leading two $p_T$-ordered jets satisfy $p_{T,1}/p_{T,2} < 1.5$; as the leading two jets are required to have similar $p_T$, this removes events with additional energetic jets.

The soft-drop algorithm is then run on the leading two jets in the selected events. Both of these jets are used for the measurement. Three different values of $\beta \in \{0, 1, 2\}$ are considered. The value of $z_{\text{cut}}$ is fixed at 0.1 so that $\log(z_{\text{cut}})$ resummation is negligible [15]. The dimensionless mass $\rho = m_{\text{soft drop}}/p_{T\text{ungroomed}}$ is the observable of interest; as the soft-drop mass is correlated with $p_T$, $\rho$ is a dimensionless quantity that only weakly depends on $p_T$. For each $\beta$ value, $\log_{10}(\rho^2)$ is constructed from the jet’s mass after the soft drop algorithm and its $p_T$ before (referred to as $p_{T\text{ungroomed}}$). The ungroomed jet $p_T$ is used because the groomed version is collinear unsafe when $\beta = 0$ [15]. The full $\log_{10}(\rho^2)$ distribution is studied, but the focus is on the resummation region $[-3.7 < \log_{10}(\rho^2) < -1.7]$, where resummation dominates over nonperturbative or fixed-order parts of the recent precision calculations; studying the distribution in log-scale allows this region to be studied more closely.

After the event selection, the data are unfolded to correct for detector effects. MC simulations are used to perform the unfolding and for comparisons with the corrected data. The unfolding procedure corrects detector-level [32] observables to particle level. The particle-level selection is defined to be as close as possible to the detector-level selection in order to minimize the size of simulation-based corrections when unfolding. Particle-level jets are clustered from simulated particles with a mean lifetime $\tau > 30$ ps excluding muons and neutrinos. These jets are built using the same algorithm as for detector-level jets, and particle-level events must pass the same dijet requirement. The experimental resolution of the $\log_{10}(\rho^2)$ distribution depends on the jet $p_T$, so the $\log_{10}(\rho^2)$ and $p_T$ distributions are simultaneously unfolded. After correcting for the acceptance of the event selection, the full two-dimensional

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distribution is unfolded using an iterative Bayesian (IB) technique [33] with four iterations as implemented in the RooUnfold framework [34]. The acceptance corrections are largely independent of \( \log_{10}(p^2) \), with a small effect below \(-3\) due to the \( \rho \neq 0 \) requirement.

Several MC simulations are used to unfold and compare to the data. Dijet events were generated at LO using PYTHIA [35] 8.186, with the \( 2 \to 2 \) matrix element (ME) convolved with the NNPDF2.3LO parton distribution function (PDF) set [36], and using the A14 [37] set of tuned PS and underlying-event model parameters. Additional radiation beyond the ME was simulated in PYTHIA 8 using the CT10 LO PDF set [41] and the default SHERPA event tune. HERWIG++ 2.7.1 [42,43] events were generated with the \( 2 \to 2 \) matrix element, convolved with the CTEQ6L1 PDF set [44] and configured with the UE-EE-5 tune [45]. Both SHERPA and HERWIG++ use angular ordering in the PS and a cluster model for hadronization [46]. All MC samples use PYTHIA 8 minimum bias events (MSTW2008LO PDF set [47] and A2 tune [48]) to

Several comparisons to data, additional dijet samples were simulated using different generators. SHERPA 2.1.1 [39] generates events using multi-leg \( 2 \to 3 \) matrix elements, which are matched to the PS following the CKKW prescription [40]. These SHERPA events were simulated using the CT10 LO PDF set [41] and the default SHERPA event tune. HERWIG++ 2.7.1 [42,43] events were generated with the \( 2 \to 2 \) matrix element, convolved with the CTEQ6L1 PDF set [44] and configured with the UE-EE-5 tune [45]. Both SHERPA and HERWIG++ use angular ordering in the PS and a cluster model for hadronization [46]. All MC samples use PYTHIA 8 minimum bias events (MSTW2008LO PDF set [47] and A2 tune [48]) to

![Graphical representation of the distributions of \( \log_{10}(p^2) \) in data compared to reconstructed detector-level (Reco.) PYTHIA, SHERPA, and HERWIG++, and particle-level (Truth) PYTHIA simulations for \( \beta = 0 \) (left), \( \beta = 1 \) (right), and \( \beta = 2 \) (bottom). The ratio of the three detector-level MC predictions to the data is shown in the middle panel, and the size of the detector → particle-level corrections for PYTHIA is shown as the ratio in the bottom panel. The error bars on the data points and in the first ratio include the experimental systematic uncertainties in the cluster energy, angular resolution, and efficiency. The distributions are normalized to the integrated cross section, \( \sigma_{\text{resum}} \), measured in the resummation region, \(-3.7 < \log_{10}(p^2) < -1.7\).](image)

FIG. 1. Distributions of \( \log_{10}(p^2) \) in data compared to reconstructed detector-level (Reco.) PYTHIA, SHERPA, and HERWIG++, and particle-level (Truth) PYTHIA simulations for \( \beta = 0 \) (left), \( \beta = 1 \) (right), and \( \beta = 2 \) (bottom). The ratio of the three detector-level MC predictions to the data is shown in the middle panel, and the size of the detector → particle-level corrections for PYTHIA is shown as the ratio in the bottom panel. The error bars on the data points and in the first ratio include the experimental systematic uncertainties in the cluster energy, angular resolution, and efficiency. The distributions are normalized to the integrated cross section, \( \sigma_{\text{resum}} \), measured in the resummation region, \(-3.7 < \log_{10}(p^2) < -1.7\).
simulate pileup. They were processed using the full ATLAS detector simulation [49] based on Geant4 [50].

Figure 1 shows the uncorrected data compared with detector-level simulation for PYTHIA, SHERPA, and HERWIG ++ as well as particle-level simulation for PYTHIA. There are substantial migrations between the detector- and particle-level distributions, which cause large off-diagonal terms in the unfolding matrix especially at low values of $\log_{10}(\rho^2)$.

Various systematic uncertainties impact the soft-drop mass distribution. The sources of uncertainty can be classified into two categories: experimental and theoretical modeling. Experimental uncertainties are due to limitations in the accuracy of the modeling of calorimeter-cell cluster energies and positions as well as their reconstructions in the accuracy of the modeling of calorimeter-cell mass distribution. The sources of uncertainty can be terms in the unfolding matrix especially at low values of particle-level distributions, which cause large off-diagonal terms in the unfolding matrix, a data-driven nonclosure technique is used to directly varying the model used to derive the response matrix. In addition to the theoretical modeling of jet fragmentation (QCD modeling). In particular, as dijet simulation is used to unfold the data, the results of the analysis are sensitive to the choice of MC generator used for this procedure. The PYTHIA generator is used for the nominal sample, and comparisons are made with SHERPA and HERWIG++. The SHERPA and HERWIG++ generators give compatible results, so only the variation with SHERPA is used as a systematic uncertainty. The impact of this uncertainty is assessed by unfolding the data with the alternative response matrix. In addition to directly varying the model used to derive the response matrix, a data-driven nonclosure technique is used to estimate the potential bias from a given choice of prior and the number of iterations in the IB method [56]. The inverse of the response matrix is applied to the particle-level spectrum, which is reweighted until the folded spectrum agrees with data. This modified detector-level distribution is unfolded with the nominal response matrix and the difference between this and the reweighted particle-level spectrum is taken as an uncertainty. Finally, the sensitivity of the unfolding procedure to pile-up is assessed by reweighting events to vary the distribution of the number of interactions in the MC simulation by 10%: the impact on the measurement is small. This is expected, since the soft-drop algorithm is designed to remove the soft, wide-angle radiation that pileup contributes.

The uncertainties are dominated by QCD modeling and the cluster energy scale. The former are largest ($\lesssim 20\%$) at low $\log_{10}(\rho^2)$ where nonperturbative effects introduce a sensitivity to the $\log_{10}(\rho^2)$ distribution prior, and are $\lesssim 10\%$ for the rest of the distribution. Cluster energy uncertainties are large ($\lesssim 5\%$) at low $\log_{10}(\rho^2)$ where the cluster multiplicity is low and also at high $\log_{10}(\rho^2)$ where the energy of the hard prongs, rather than their opening angle, dominates the mass resolution. Other sources of uncertainty are typically below 5% across the entire distribution. A summary of the relative sizes of the various systematic uncertainties for $\beta = 0$ is shown in Fig. 2. The relative sizes of the different sources of systematic uncertainty are similar for $\beta = 1$ and $\beta = 2$, except that the large uncertainty at low $\log_{10}(\rho^2)$ values spans a larger range.

The unfolded data are shown in Fig. 3. They are compared to the predictions of the PYTHIA, SHERPA, and HERWIG++ generators, as well as the NLO + NLL prediction from Refs. [15,16] and the LO + NNLL prediction from Refs. [17,18]. The (N)NLL calculations use NLOjet++ [57,58] (MG5_aMC [59]) with the CT14nlo [60] (MSTW2008LO) PDF set for matrix element calculations. The distributions are normalized to the integrated

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Relative Uncertainty} & \textbf{MC statistical error} & \textbf{Data statistical error} & \textbf{QCD Modeling} \\
\hline
\textbf{Total uncertainty} & \textbf{Nonclosure} & \textbf{Cluster angular resolution} & \textbf{Cluster energy scale shift} \\
\hline
\textbf{Soft drop, $\beta = 0$, $z_{cut} = 0.1$} & \textbf{anti-$k_T$, $R=0.8$, $p_T^{\text{lead}} > 600$ GeV} & \textbf{Cluster energy scale matching} & \textbf{Pileup modeling} \\
\hline
\end{tabular}
\caption{Relative uncertainties from Refs. [15,16] and the LO + NLL prediction from Refs. [17,18]. The (N)NLL calculations use NLOjet++ [57,58] (MG5_aMC [59]) with the CT14nlo [60] (MSTW2008LO) PDF set for matrix element calculations. The distributions are normalized to the integrated}
\end{table}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{The breakdown of systematic and statistical uncertainties as a function of $\log_{10}(\rho^2)$ for $\beta = 0$.}
\end{figure}
cross section, $\sigma_{\text{resum}}$, measured in the resummation region, $-3.7 < \log_{10}(\rho^2) < -1.7$. The uncertainties due to the analytical calculation come from independently varying each of the renormalization, factorization, and resummation scales by factors of 2 and 1/2. The NLO + NLL calculation is also given with nonperturbative (NP) corrections based on the average of various MC models with NP effects turned on and off; the envelope of predictions is added as an uncertainty [15]. The LO + NNLL predictions do not contain NP effects, but the open markers in Fig. 3 indicate where NP are expected to be large ("large NP effects").

The MC predictions and the analytical calculations are expected to be accurate in different regions of $\log_{10}(\rho^2)$ [15,17,18]. In general, nonperturbative effects are large for

FIG. 3. The unfolded $\log_{10}(\rho^2)$ distribution for anti-$k_T$ $R = 0.8$ jets with $p_T^{\text{had}} > 600$ GeV, after the soft-drop algorithm is applied for $\beta \in \{0, 1, 2\}$, in data compared to PYTHIA, SHERPA, and HERWIG++ particle-level (left), and NLO + NLL (+NP) [15] and LO + NNLL [17,18] theory predictions (right). The LO + NNLL calculation does not have nonperturbative corrections; the region where these are expected to be large is shown in an open marker (but no correction is applied), while regions where they are expected to be small are shown with a filled marker. All uncertainties described in the text are shown on the data; the uncertainties from the calculations are shown on each one. The distributions are normalized to the integrated cross section, $\sigma_{\text{resum}}$, measured in the resummation region, $-3.7 < \log_{10}(\rho^2) < -1.7$. The NLO + NLL + NP cross section in this resummation regime is 0.14, 0.19, and 0.21 nb for $\beta = 0, 1, 2$, respectively [15].
log_{10}(\rho^2) < -3.7 (where small-angle or soft gluon emissions dominate) and small for -3.7 < log_{10}(\rho^2) < -1.7 where resummation dominates. Fixed, higher-order corrections are expected to be important for log_{10}(\rho^2) > -1.7, where large-angle gluon emission can play an important role. This implies that the region -3.7 < log_{10}(\rho^2) < -1.7 (the resummation region) should have the most reliable predictions for both the MC generators and the LO + NNLL analytical calculation, while the NLO + NLL calculation should also be accurate for log_{10}(\rho^2) > -1.7. For all values of \beta, the measured and predicted shapes agree well in the resummation region, and the data and NLO + NLL prediction continue to agree well at higher values of log_{10}(\rho^2). At more negative values of log_{10}(\rho^2), nonperturbative effects lead to distinctly different predictions between the MC generators and the calculations without NP corrections; the data fall below the predictions for all \beta values. Interestingly, the NNLL calculation is not everywhere a better model of the data than the NLL calculation in the resummation regime and NP effects can also be comparable to the higher order resummation calculation in the resummation regime and NP effects. Therefore, improved precision for the future will require will require a careful comparative analysis of the different perturbative calculations as well as a deeper and possibly analytic understanding of NP effects.

As \beta increases, the fraction of radiation removed by soft-drop grooming decreases and the impact of nonperturbative effects grows larger \cite{17,18}, so the range over which the analytical calculations are accurate also decreases. The degree of agreement between data and all the calculations for log_{10}(\rho^2) < -3 does substantially worsen for \beta \in \{1,2\}, especially when NP corrections are not included. Agreement between the data and the MC generators remains generally within uncertainties for all values of \beta. Digitized versions of the results, along with versions binned in jet p_T can be found at Ref. \cite{61}.

In summary, a measurement of the soft-drop jet mass is reported. The measurement provides a comparison of the internal properties of jets between 32.9 fb^{-1} of 13 TeV pp collision data collected by the ATLAS detector at the LHC and precision QCD calculations accurate beyond leading logarithm. Where the calculations are well defined perturbatively, they agree well with the data; in regions where nonperturbative effects are expected to be significant, the calculations disagree with the data and the predictions from MC simulation are better able to reproduce the data. The dijet cross section is presented as a normalized fiducial dijet differential cross section as a function of the log_{10}(\rho^2) for each jet, allowing the results to be used to constrain future calculations and MC generator predictions.

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\begin{thebibliography}{12}
\item There are nearly 100 public search results from ATLAS and CMS as well as an even larger number of phenomenological proposals to use jet substructure to enhance various searches. See e.g., Refs. \cite{2,3} for the first phenomenological proposals and Refs. \cite{4,5,6,7} for representative ATLAS and CMS performance studies.


\end{thebibliography}
For a detailed and pedagogical discussion, see e.g., G. P. Salam, Towards jetography, Eur. Phys. J. C 67, 637 (2010).


ATLAS uses a right-handed coordinate system with its origin at the interaction point in the center of the detector. Cylindrical coordinates $r, \phi$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam axis. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta = -\ln \tan(\theta/2)$. The rapidity, differences of which are invariant under longitudinal boosts also for massive particles, is defined as $y = \frac{1}{2} \ln[(E + p_z)/(E - p_z)]$.


Resulting from quantum chromodynamic coherence; for further details, see e.g., R. K. Ellis, W. J. Stirling, and B. R. Webber, QCD and Collider Physics, (Cambridge University Press, Cambridge, UK, 1996).


Detector level refers to the measured outputs of the detector; particle level refers to the particles that interact with the detector.


(The ATLAS Collaboration)

1Department of Physics, University of Adelaide, Adelaide, Australia
2Physics Department, SUNY Albany, Albany, New York, USA
3Department of Physics, University of Alberta, Edmonton, Alberta, Canada
4Department of Physics, Ankara University, Ankara, Turkey
4aIstanbul Aydin University, Istanbul, Turkey
4bGraduate School of Natural Sciences, Anadolu University, Eskisehir, Turkey
4cDivision of Physics, TOBB University of Economics and Technology, Ankara, Turkey
5LAPP, CNRS/IN2P3 and Université Savoie Mont Blanc, Annecy-le-Vieux, France
6High Energy Physics Division, Argonne National Laboratory, Argonne, Illinois, USA
7Department of Physics, University of Arizona, Tucson, Arizona, USA
8Department of Physics, The University of Texas at Arlington, Arlington, Texas, USA
9Physics Department, National and Kapodistrian University of Athens, Athens, Greece
10Physics Department, National Technical University of Athens, Zografou, Greece
11Department of Physics, The University of Texas at Austin, Austin, Texas, USA
12Institute of Physics, Azerbaijan Academy of Sciences, Baku, Azerbaijan
13Institut de Física d’Altes Energies (IFAE), The Barcelona Institute of Science and Technology, Barcelona, Spain
14Institute of Physics, University of Belgrade, Belgrade, Serbia
15Department for Physics and Technology, University of Bergen, Bergen, Norway
16Physics Division, Lawrence Berkeley National Laboratory and University of California, Berkeley, California, USA
17Department of Physics, Humboldt University, Berlin, Germany
18Albert Einstein Center for Fundamental Physics and Laboratory for High Energy Physics, University of Bern, Bern, Switzerland
19School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom
20aDepartment of Physics, Bogazici University, Istanbul, Turkey
20bDepartment of Physics Engineering, Gaziantep University, Gaziantep, Turkey
21Centro de Investigaciones, Universidad Antonio Narino, Bogota, Colombia
22INFN Sezione di Bologna, Bologna, Italy
22aDipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy
23Physikalisches Institut, Universität Bonn, Bonn, Germany
24Department of Physics, Boston University, Boston, Massachusetts, USA

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Department of Physics, Brandeis University, Waltham, Massachusetts, USA
26a Universidade Federal do Rio De Janeiro COPPE/EE/IF, Rio de Janeiro, Brazil
26b Electrical Circuits Department, Federal University of Juiz de Fora (UFJF), Juiz de Fora, Brazil
26c Federal University of Sao Joao del Rei (UFSJ), Sao Joao del Rei, Brazil
26d Instituto de Fisica, Universidade de Sao Paulo, Sao Paulo, Brazil
27 Physics Department, Brookhaven National Laboratory, Upton, New York, USA
28a Transilvania University of Brasov, Brasov, Romania
28b Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania
28c Department of Physics, Alexandru Ioan Cuza University of Iasi, Iasi, Romania
28d National Institute for Research and Development of Isotopic and Molecular Technologies, Physics Department, Cluj Napoca, Romania
28e University Politehnica Bucharest, Bucharest, Romania
28f West University in Timisoara, Timisoara, Romania
29 Departamento de Fisica, Universidad de Buenos Aires, Buenos Aires, Argentina
30 Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom
31 Department of Physics, Carleton University, Ottawa, Ontario, Canada
32 CERN, Geneva, Switzerland
33 Enrico Fermi Institute, University of Chicago, Chicago, Illinois, USA
34a Departamento de Física, Pontificia Universidad Católica de Chile, Santiago, Chile
34b Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile
35a Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China
35b Department of Physics, Nanjing University, Jiangsu, China
35c Physics Department, Tsinghua University, Beijing 100084, China
35d University of Chinese Academy of Science (UCAS), Beijing, China
36a Department of Modern Physics and State Key Laboratory of Particle Detection and Electronics, University of Science and Technology of China, Anhui, China
36b School of Physics, Shandong University, Shandong, China
36c Department of Physics and Astronomy, Key Laboratory for Particle Physics, Astrophysics and Cosmology, Ministry of Education; Shanghai Key Laboratory for Particle Physics and Cosmology, Shanghai Jiao Tong University, Tsung-Dao Lee Institute, China
37 Université Clermont Auvergne, CNRS/IN2P3, LPC, Clermont-Ferrand, France
38 Nevis Laboratory, Columbia University, Irvington, New York, USA
39 Niels Bohr Institute, University of Copenhagen, Kobenhavn, Denmark
40a INFN Gruppo Collegato di Cosenza, Laboratori Nazionali di Frascati, Rende, Italy
40b Dipartimento di Fisica, Università della Calabria, Rende, Italy
41a AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland
41b Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland
42 Institute of Nuclear Physics Polish Academy of Sciences, Krakow, Poland
43 Physics Department, Southern Methodist University, Dallas, Texas, USA
44 Physics Department, University of Texas at Dallas, Richardson, Texas, USA
45 DESY, Hamburg and Zeuthen, Germany
46 Lehrstuhl für Experimentelle Physik IV, Technische Universität Dortmund, Dortmund, Germany
47 Institut für Kern- und Teilchenphysik, Technische Universität Dresden, Dresden, Germany
48 Department of Physics, Duke University, Durham, North Carolina, USA
49 SUPA—School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom
50 INFN e Laboratori Nazionali di Frascati, Frascati, Italy
51 Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany
52 Département de Physique Nucléaire et Corpusculaire, Université de Genève, Geneva, Switzerland
53 INFN Sezione di Genova, Genova, Italy
54a Dipartimento di Fisica, Università di Genova, Genova, Italy
54b E. Andronikashvili Institute of Physics, Iv. Javakhishvili Tbilisi State University, Tbilisi, Georgia
54c High Energy Physics Institute, Tbilisi State University, Tbilisi, Georgia
55 a II Physikalisches Institut, Justus-Liebig-Universität Giessen, Giessen, Germany
56b SUPA—School of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom
57 a II Physikalisches Institut, Georg-August-Universität, Göttingen, Germany
58 Laboratoire de Physique Subatomique et de Cosmologie, Université Grenoble-Alpes, CNRS/IN2P3, Grenoble, France
59 Laboratory for Particle Physics and Cosmology, Harvard University, Cambridge, Massachusetts, USA
60 Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
60a Physikalisches Institut, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany
61 Faculty of Applied Information Science, Hiroshima Institute of Technology, Hiroshima, Japan
62 Department of Physics, The Chinese University of Hong Kong, Shatin, N. T., Hong Kong, China
Department of Physics, Oklahoma State University, Stillwater, Oklahoma, USA

Center for High Energy Physics, University of Oregon, Eugene, Oregon, USA

LAL, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France

Graduate School of Science, Osaka University, Osaka, Japan

Department of Physics, University of Oslo, Oslo, Norway

Department of Physics, Oxford University, Oxford, United Kingdom

INFN Sezione di Pavia, Pavia, Italy

Dipartimento di Fisica, Università di Pavia, Pavia, Italy

National Research Centre "Kurchatov Institute" B. P.Konstantinov Petersburg Nuclear Physics Institute, St. Petersburg, Russia

INFN Sezione di Pisa, Pisa, Italy

Dipartimento di Fisica E. Fermi, Università di Pisa, Pisa, Italy

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania, USA

Laboratório de Instrumentação e Física Experimental de Partículas—LIP, Lisboa, Portugal

Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

Department of Physics, University of Coimbra, Coimbra, Portugal

Centro de Física Nuclear da Universidade de Lisboa, Lisboa, Portugal

Departamento de Física, Universidade do Minho, Braga, Portugal

Departamento de Física Teorica y del Cosmos, Universidad de Granada, Granada, Spain

Dep Física and CEFITEC of Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, Caparica, Portugal

Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic

Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

State Research Center Institute for High Energy Physics (Protvino), NRC KI, Russia

Particle Physics Department, Rutherford Appleton Laboratory, Didcot, United Kingdom

INFN Sezione di Roma, Roma, Italy

INFN Sezione di Roma Tor Vergata, Roma, Italy

INFN Sezione di Roma Tre, Roma, Italy

Faculté des Sciences Ain Chock, Réseau Universitaire de Physique des Hautes Energies—Université Hassan II, Casablanca, Morocco

Centre National de l’Energie des Sciences Techniques Nucleaires, Rabat, Morocco

Faculté des Sciences Semlalia, Université Cadi Ayyad, LPHEA-Marrakech, Morocco

Faculté des Sciences, Université Mohamed Premier and LPTPM, Oujda, Morocco

Faculté des sciences, Université Mohammed V, Rabat, Morocco

DSM/IRFU (Institut de Recherches sur les Lois Fondamentales de l’Univers), CEA Saclay (Commissariat à l’Energie Atomique et aux Energies Alternatives), Gif-sur-Yvette, France

Santa Cruz Institute for Particle Physics, University of California Santa Cruz, Santa Cruz, California, USA

Department of Physics, University of Washington, Seattle, Washington, USA

Department of Physics and Astronomy, University of Sheffield, Sheffield, United Kingdom

Department of Physics, Shinshu University, Nagano, Japan

Department Physik, Universität Siegen, Siegen, Germany

Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada

SLAC National Accelerator Laboratory, Stanford, California, USA

Faculty of Mathematics, Physics & Informatics, Comenius University, Bratislava, Slovak Republic

Department of Subnuclear Physics, Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovak Republic

Department of Physics, University of Cape Town, Cape Town, South Africa

Department of Physics, University of Johannesburg, Johannesburg, South Africa

School of Physics, University of the Witwatersrand, Johannesburg, South Africa

Department of Physics, Stockholm University, Sweden

The Oskar Klein Centre, Stockholm, Sweden

Physics Department, Royal Institute of Technology, Stockholm, Sweden

Departments of Physics & Astronomy and Chemistry, Stony Brook University, Stony Brook, New York, USA

Department of Physics and Astronomy, University of Sussex, Brighton, United Kingdom

School of Physics, University of Sydney, Sydney, Australia
Also at LAL, Univ. Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, Orsay, France.
Also at Graduate School of Science, Osaka University, Osaka, Japan.
Also at Fakultät für Mathematik und Physik, Albert-Ludwigs-Universität, Freiburg, Germany.
Also at Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen/Nikhef, Nijmegen, Netherlands.
Also at Department of Physics, The University of Texas at Austin, Austin, TX, USA.
Also at Institute of Theoretical Physics, Ilia State University, Tbilisi, Georgia.
Also at CERN, Geneva, Switzerland.
Also at Georgian Technical University (GTU), Tbilisi, Georgia.
Also at Ochadai Academic Production, Ochanomizu University, Tokyo, Japan.
Also at Manhattan College, New York, NY, USA.
Also at The City College of New York, New York, NY, USA.
Also at Departamento de Fisica Teorica y del Cosmos, Universidad de Granada, Granada, Spain.
Also at Department of Physics, California State University, Sacramento, CA, USA.
Also at Moscow Institute of Physics and Technology State University, Dolgoprudny, Russia.
Also at Departement de Physique Nucleaire et Corpusculaire, Université de Genève, Geneva, Switzerland.
Also at Institut de Física d’Altes Energies (IFAE), The Barcelona Institute of Science and Technology, Barcelona, Spain.
Also at School of Physics, Sun Yat-sen University, Guangzhou, China.
Also at Institute for Nuclear Research and Nuclear Energy (INRNE) of the Bulgarian Academy of Sciences, Sofia, Bulgaria.
Also at Faculty of Physics, M. V. Lomonosov Moscow State University, Moscow, Russia.
Also at National Research Nuclear University MEPhI, Moscow, Russia.
Also at Department of Physics, Stanford University, Stanford, CA, USA.
Also at Institute for Particle and Nuclear Physics, Wigner Research Centre for Physics, Budapest, Hungary.
Also at Giresun University, Faculty of Engineering, Turkey.
Also at CPPM, Aix-Marseille Université and CNRS/IN2P3, Marseille, France.
Also at Department of Physics, Nanjing University, Jiangsu, China.
Also at Institute of Physics, Academia Sinica, Taipei, Taiwan.
Also at University of Malaya, Department of Physics, Kuala Lumpur, Malaysia.