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Letter

Characterization of the quantum state of top quark pairs produced in proton-proton collisions at $\sqrt{s} = 13$ TeV using the beam and helicity bases

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Measurements of the spin correlation coefficients in the beam basis are presented for top quark-antiquark ($t\bar{t}$) systems produced in proton-proton collisions at $\sqrt{s} = 13$ TeV collected by the CMS experiment in 2016–2018, and corresponding to an integrated luminosity of 138 fb^{-1}. The $t\bar{t}$ system is reconstructed from final states containing an electron or muon and jets. Together with the previously reported results in the helicity basis, these measurements are used to decompose the system into the Bell and spin eigenstates in various kinematic regions. The spin correlation coefficients are also used to evaluate properties of the $t\bar{t}$ quantum state, such as the purity, von Neumann entropy, and entanglement. All results are consistent with standard model predictions.

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The top quark is the most massive known fundamental particle, with a lifetime on the order of 10^{-25} s. This lifetime is shorter than both the quantum chromodynamics (QCD) hadronization timescale $1/\Lambda_{\text{QCD}} \approx 10^{-24}$ s and the spin decorrelation timescale $m_t/\Lambda^2_{\text{QCD}} \approx 10^{-21}$ s, where m_t denotes the top quark mass [1,2]. Consequently, the top quark spin information is preserved in the angular distribution of its decay products, which makes top quark-antiquark ($t\bar{t}$) pairs excellent probes for studying polarization and spin correlations [3,4]. The spins of the top quarks are expected to be strongly correlated [5], which can translate into the $t\bar{t}$ pair having nonclassical correlations—i.e., entangled top quarks.

The recent measurements of polarization and spin correlations in the helicity basis, as well as the observation of entanglement, by the ATLAS [6] and CMS [7,8] Collaborations, mark a significant step in the characterization of the $t\bar{t}$ system. In this paper, we extend the measurements of the spin correlation matrix to the beam basis. While the helicity basis is particularly suited for analyzing the spin correlations and entanglement at high invariant masses of the $t\bar{t}$ system, $m(t\bar{t})$, the beam basis provides complementary sensitivity to the measurements near the production threshold [9,10].

The CMS apparatus [11,12] is a multipurpose, nearly hermetic detector, designed to trigger on [13–15] and identify electrons, muons, photons, and hadrons [16–18]. A global algorithm [19] aims to reconstruct all individual particles in an event, combining information provided by the all-silicon tracker and by the crystal electromagnetic and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from the gas-ionization muon detectors interleaved with the layers of the flux-return yoke outside the solenoid. The reconstructed particles are used to build τ leptons, jets, and missing transverse momentum [20–22].

Collision data taken from 2016 to 2018 and corresponding to 138 fb^{-1} [23–25] have been used for the measurements reported in Ref. [8]. Following the conventions introduced in Ref. [4], these measurements were used to derive the results in the helicity basis presented in this article. It should be noted that this definition of the helicity basis includes a discrete rotation of π around the k axis if $\theta > \pi/2$, where k and θ are the top quark's direction vector and its scattering angle, respectively, in the $t\bar{t}$ rest frame. This convention was introduced to account for the Bose-Einstein symmetry of the gluon-gluon (gg) initial state.

In the beam basis, the z axis is aligned with the proton beams, with fixed x and y axes given by the CMS coordinate system—i.e., the x axis pointing toward the center of the LHC ring, and the y axis oriented vertically upward [11]. Similarly to the definition of the helicity basis, the top quarks and their decay products are actively boosted from the laboratory frame into the $t\bar{t}$ rest frame, followed by an active boost of the top (anti)quark decay products from the $t\bar{t}$ rest frame into their parent's rest frame, where active boosts, used in the definition of both bases, imply Lorentz transformations of the particles' four-momenta while the coordinate systems remain unchanged. As a consequence of the symmetries around the beam axis and between the

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incoming protons, the spin correlation matrix C_{ij} is diagonal with $C_\perp = C_{xx} = C_{yy}$ and $C_\parallel = C_{zz}$, and the polarization coefficients P_i and $\bar{P}_i$ of the top quark and antiquark, respectively, are equal to zero [26]. For the beam basis, the additional rotation to account for the Bose-Einstein symmetry is not applied. Since the axes in the helicity basis are defined eventwise based on the top quark direction, it is necessary to reanalyze each selected event to obtain the results in the beam basis.

At the CERN LHC, the $t\bar{t}$ system is produced predominantly via gg fusion. Quark-antiquark annihilation also contributes, accounting for approximately 10% of the production rate on average. Near the production threshold, the $gg \to t\bar{t}$ events are produced predominantly in a spin-singlet configuration. In contrast, at high transverse momentum of the top quark, $p_\mathrm{T}(t)$, the production approaches a spin-triplet state [26]. The contributions of individual states can be evaluated from the density matrix ρ, which can be written in the Fano-Bloch decomposition [27] as

$$\rho = \frac{1}{4}\left(I \otimes I + \sum_i P_i \sigma_i \otimes I + \sum_j \bar{P}_j I \otimes \sigma_j - \sum_{ij} C_{ij} \sigma_i \otimes \sigma_j\right), \tag{1}$$

where I is the 2×2 identity matrix and σ_i are Pauli matrices.

To characterize the quantum state, we perform the eigenvector decomposition of ρ and identify the eigenvectors in the helicity basis with the Bell states [28]

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle),$$
$$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle), \tag{2}$$

and in the beam basis with the spin states: singlet $|\Psi^-\rangle$ (pseudoscalar) and triplet $|\uparrow\uparrow\rangle$, $|\Psi^+\rangle$, $|\downarrow\downarrow\rangle$ (vector).

For the spin quantization axis, we choose the k direction in the helicity basis and the z direction in the beam basis. The contributions of the individual states are evaluated as the expectation value of ρ for the corresponding state $|\psi_i\rangle$

$$\langle\psi_i|\rho|\psi_i\rangle. \tag{3}$$

In quantum mechanics, the purity is defined as

$$\gamma(\rho) = \mathrm{Tr}(\rho^2), \tag{4}$$

which measures how mixed a quantum state is. For a pure state, $\rho^2 = \rho$, and thus purity equals unity. In contrast, for mixed states, $\mathrm{Tr}(\rho^2) < 1$.

The von Neumann entropy $S(\rho)$, which is a quantum-mechanical generalization of the Shannon entropy [29], characterizes the amount of uncertainty about the value of a random variable, and is defined as

$$S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho). \tag{5}$$

The entropy is zero only for pure states and reaches its highest value for the maximally mixed states, following the intuition of the classical entropy. Since the $t\bar{t}$ system involves two spin-1/2 particles, the entropy range is $0 < S(\rho) < 2$. Purity and entropy quantify whether the $t\bar{t}$ system is described predominantly by a single state or by a mixture of several states. High purity (or low entropy) indicates that a single state predominantly contributes, whereas low purity (or high entropy) signals that several states contribute comparably.

A sufficient condition for the entanglement based on the Peres-Horodecki criterion [30,31] is given by the entanglement marker [26,32]

$$\Delta_\mathrm{E} = C_{11} + |C_{22} + C_{33}| > 1, \tag{6}$$

where the indices (1, 2, 3) of the diagonal elements of the spin correlation matrix refer to (x, y, z) in the beam and (n, r, k) in the helicity basis. This condition applies under the assumption that the $t\bar{t}$ state is fully described by quantum mechanics [33,34].

We present the characterization of the quantum properties of the $t\bar{t}$ system in bins of $m(t\bar{t})$ vs $|\cos(\theta)|$ and $p_\mathrm{T}(t)$ vs $|\cos(\theta)|$. In the helicity basis, the polarizations and spin correlations are directly taken from Ref. [8], while in the beam basis, the measurements of $C_\perp$ and $C_\parallel$ are new results. This analysis uses the same method introduced in Ref. [8], including the object selection, reconstruction of the $t\bar{t}$ system, and treatment of systematic uncertainties. The polarization and spin correlation coefficients are determined from a template fit to the angular distributions of the $t\bar{t}$ decay products. Since only $C_\perp$ and $C_\parallel$ can be nonzero in the beam basis, all other coefficients are fixed to zero in the fit.

The results are compared to the values predicted by the standard model using the Monte Carlo–simulated samples described in Ref. [8]. These predictions are obtained using the matrix element (ME) event generator POWHEG v2 [35–37] subsequently combined with the parton shower simulation from PYTHIA 8.240 [38], using the underlying event tune CP5 [39]. For these predictions, we evaluate the ME scale and parton distribution function (PDF) uncertainties. In addition, the measured coefficients in the beam basis are compared to the predictions obtained using POWHEG + Herwig 7.1 [40] with tune CH3 [41], and MINNLO + PYTHIA, a $t\bar{t}$ sample at next-to-next-to-leading order (NNLO) QCD generated with POWHEG MINNLO [42] in combination with the CP5 PYTHIA tune. Tabulated results for all figures, including the $p_\mathrm{T}(t)$ vs $|\cos(\theta)|$ measurements, are provided in the HEPData record for this analysis [43].

In Fig. 1, we present the measured spin correlation coefficients in the beam basis in $m(t\bar{t})$ vs $|\cos(\theta)|$ and $p_\mathrm{T}(t)$ vs $|\cos(\theta)|$ bins. The statistical uncertainties shown as the

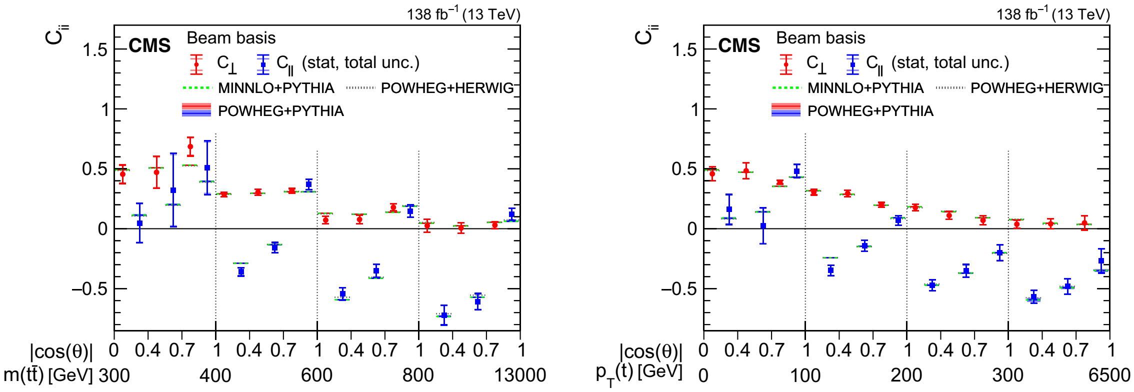

FIG. 1. Results of the spin correlation coefficients in bins of $m(t\bar{t})$ vs $|\cos(\theta)|$ (left) and $p_{\mathrm{T}}(t)$ vs $|\cos(\theta)|$ (right) in the beam basis. The measurements (markers) are shown with the statistical (inner error bars) and total (outer error bars) uncertainties and compared to the predictions from POWHEG + Herwig, MINNLO + PYTHIA, and POWHEG + PYTHIA. The POWHEG + PYTHIA prediction is displayed with the ME scale and PDF uncertainties.

inner error bars dominate and nearly coincide with the total uncertainties shown as the outer error bars. From χ^2 tests comparing measured coefficients to the various predictions, the p-values fall within 0.22–0.34 (0.70–0.79) for the $m(t\bar{t})$ vs $|\cos(\theta)|$ [$p_{\mathrm{T}}(t)$ vs $|\cos(\theta)|$] measurements, indicating agreement in all cases. These p-values are obtained by taking into account the full experimental covariance matrix. The corresponding coefficients for the helicity basis can be found in Ref. [8].

The uncertainties in the observables derived from the polarization and spin correlation coefficients are evaluated using pseudoexperiments, which are generated by sampling from a multivariate normal distribution defined by the measured central values and the covariance matrix of the coefficients. To ensure physically meaningful results, pseudoexperiments are rejected if they lead to negative eigenvalues of the density matrix, or if any of the spin correlation coefficients satisfy $|C_{ij}| > 1$. Potential biases in

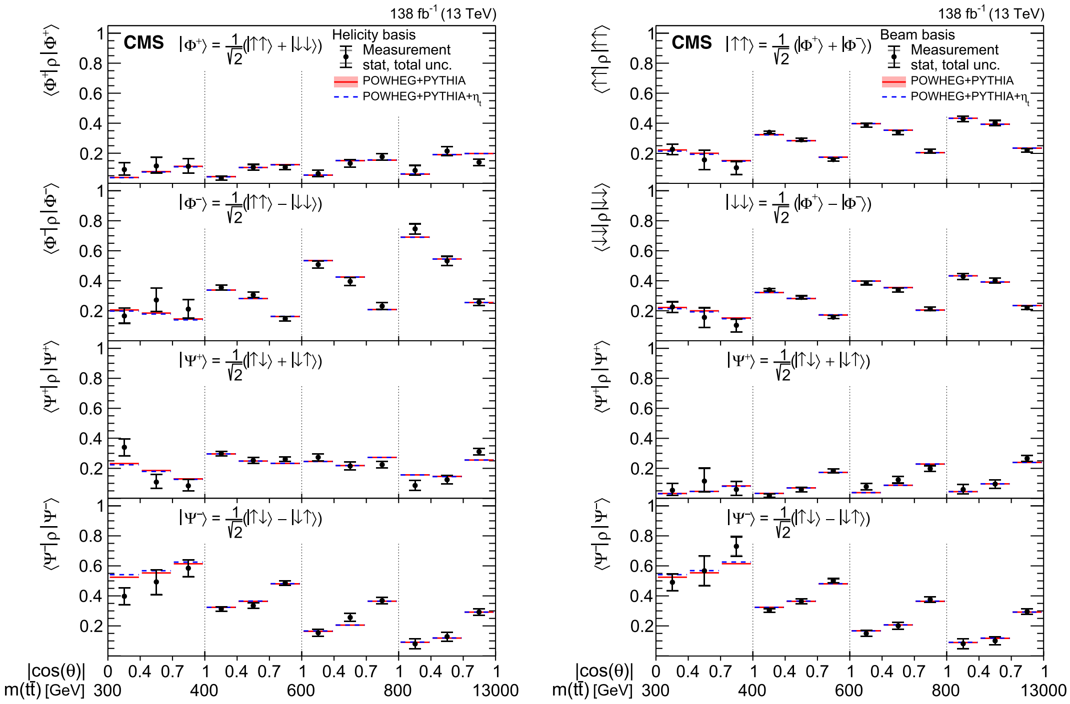

FIG. 2. Results of the state decomposition in terms of the Bell and spin states in bins of $m(t\bar{t})$ vs $|\cos(\theta)|$ in the helicity (left) and beam (right) basis. The measurements (markers) are shown with the statistical (inner error bars) and total (outer error bars) uncertainties and compared to the predictions from POWHEG + PYTHIA and POWHEG + PYTHIA + η_t. The POWHEG + PYTHIA prediction is displayed with the ME scale and PDF uncertainties.

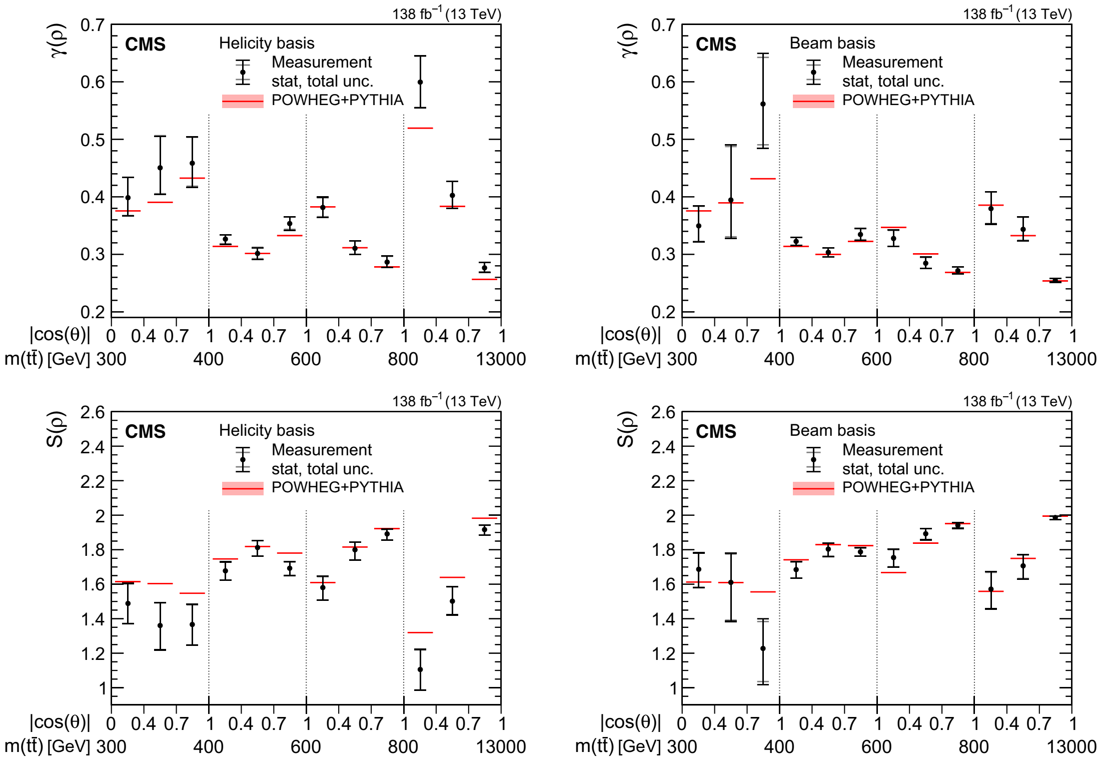

FIG. 3. Results of the purity $\gamma(\rho)$ (upper) and entropy $S(\rho)$ (lower) measurements in bins of $m(t\bar{t})$ vs $|\cos(\theta)|$ in the helicity (left) and beam (right) basis. The measurements (markers) are shown with the statistical (inner error bars) and total (outer error bars) uncertainties and compared to the predictions from POWHEG + PYTHIA, shown with the ME scale and PDF uncertainties.

the pseudoexperiments have been evaluated and are negligible relative to the measurement uncertainties. The statistical uncertainties dominate and nearly coincide with the total uncertainties in all the observables.

The eigenvector decomposition of ρ is shown in Fig. 2 and compared to the POWHEG + PYTHIA simulation. In the helicity basis for $m(t\bar{t}) > 800$ GeV and $|\cos(\theta)| < 0.4$, we see the largest individual contribution (~70%) of the $|\Phi^-\rangle$ Bell state. In both the helicity and the beam basis, high contributions (60%–70%) of the $|\Psi^-\rangle$ pseudoscalar state are observed near the $t\bar{t}$ production threshold for $m(t\bar{t}) < 400$ GeV. Although the short lifetime of the top quark prevents the formation of long-lived $t\bar{t}$ bound states, nonrelativistic QCD calculations predict bound-state-like enhancements near the $t\bar{t}$ production threshold [44–48]. These effects are simulated using MadGraph5_aMC@NLO + PYTHIA as a pseudoscalar particle, η_t, produced via gg fusion with a mass of 343 GeV and a width equal to twice

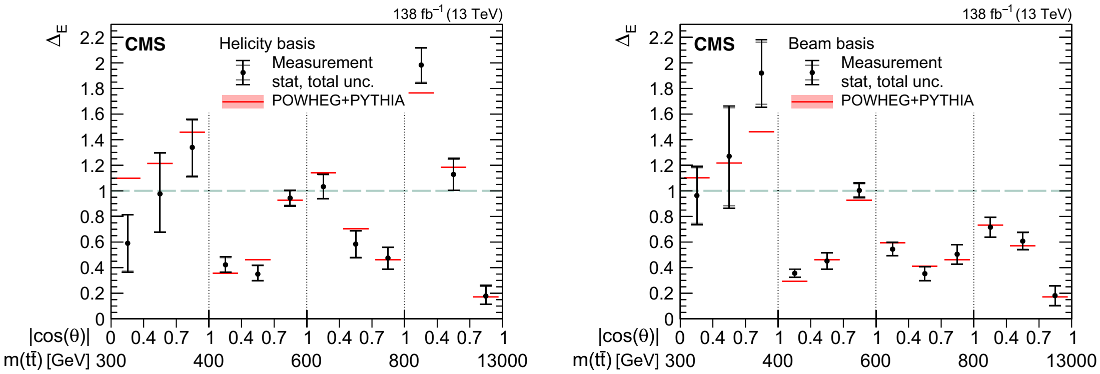

FIG. 4. Results of the entanglement marker Δ_E measurements in bins of $m(t\bar{t})$ vs $|\cos(\theta)|$ in the helicity (left) and beam (right) basis. The measurements (markers) are shown with the statistical (inner error bars) and total (outer error bars) uncertainties and compared to the predictions from POWHEG + PYTHIA, shown with the ME scale and PDF uncertainties. The dashed green line represents the lower bound for entangled states.

the top quark width, which decays as $\eta_t \to W^+ b W^- \bar{b}$ with the same spin correlations as $t\bar{t}$ pairs in a pure $|\Psi^-\rangle$ spin-singlet state. This simulation is normalized to the cross section of 6.43 pb from Ref. [48] and added to the nominal POWHEG + PYTHIA prediction as an additional comparison in Fig. 2. The expected enhancement of the $|\Psi^-\rangle$ state caused by the η_t contribution near the threshold is smaller than the uncertainty, hence the two models cannot be distinguished by these measurements. The contributions of the triplet states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are equal in the beam basis because of the symmetry between the incoming protons.

In Fig. 3, the extracted purity $\gamma(\rho)$ and entropy $S(\rho)$ values are shown in the helicity and beam bases. Overall, we observe agreement with the standard model predictions for both $\gamma(\rho)$ and $S(\rho)$. The maximum deviations are found in the helicity basis for the lowest and highest $m(t\bar{t})$ bins, where a slightly higher $\gamma(\rho)$ and lower $S(\rho)$ than expected are observed. However, the differences are all within 2 standard deviations. In the helicity basis, $\gamma(\rho)$ is highest at high $m(t\bar{t})$ and low $|\cos(\theta)|$, where $S(\rho)$ reaches its minimum value. In the beam basis, $\gamma(\rho)$ is highest at low $m(t\bar{t})$ and high $|\cos(\theta)|$, which corresponds to the region of lowest $S(\rho)$. As expected, $S(\rho)$ is nonzero across all bins. We note that in Fig. 2 for both bases in the $m(t\bar{t}) > 800$ GeV, $|\cos(\theta)| > 0.7$ bin, all the Bell or spin states make similar contributions, which is reflected in the purity being the lowest in this bin.

In Fig. 4, the entanglement marker Δ_{E} values are shown in the helicity and beam bases. The dashed green line represents the entanglement criterion: states with $\Delta_{\mathrm{E}} > 1$ are entangled. In the helicity basis, the Δ_{E} is highest at high $m(t\bar{t})$ and low $|\cos(\theta)|$, where the significance of entanglement exceeds 5 standard deviations, as was already reported in Ref. [8]. In the beam basis, we find evidence of entanglement in the threshold region, with a significance of greater than 3 standard deviations for $|\cos(\theta)| > 0.7$.

In summary, the spin correlation measurements of the top quark-antiquark ($t\bar{t}$) system from Ref. [8] are extended to include results in the beam basis for the first time. This is done with bins in two dimensions, comprising the top quark scattering angle and either the invariant mass of the $t\bar{t}$ system or the transverse momentum of the top quark, using proton-proton collisions at $\sqrt{s} = 13$ TeV recorded by the CMS experiment at the LHC, corresponding to an integrated luminosity of 138 fb^{-1}. The density matrix is decomposed into eigenstates, which are identified as Bell states in the helicity basis and spin states in the beam basis. We also present the first experimental results for the purity, von Neumann entropy, and entanglement of the $t\bar{t}$ system in both bases. All the measurements are consistent with standard model expectations.

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Data availability. Release and preservation of data used by the CMS Collaboration as the basis for publications is guided by the CMS data preservation, reuse, and open access policy [49].

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