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Observation of structures in the $J/\psi + \psi(2S)$ mass spectrum with the ATLAS detector

The ATLAS Collaboration

A search for resonant structures in the $J/\psi + \psi(2S)$ mass spectrum is performed using proton–proton collision data at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 140 fb^{-1} , recorded by the ATLAS experiment at the LHC. The decay channels of $J/\psi + \psi(2S) \rightarrow 4\mu$ and $J/\psi + \psi(2S) \rightarrow 4\mu + 2\pi$ are analyzed. An excess near 6.9 GeV is observed in both channels with a combined significance of 8.9σ . No significant signal is observed near 7.2 GeV, and an upper limit on its yield relative to $X(6900)$ is provided. A simultaneous fit with the di- J/ψ channel is carried out under assumptions regarding the resonance interferences, yielding a ratio of the partial decay widths between the $J/\psi + \psi(2S)$ and di- J/ψ channels of $1.08 \pm 0.20^{+0.40}_{-0.17}$ for the resonance near 6.9 GeV.

The study of tetraquark states ($qq\bar{q}\bar{q}$) can further our understanding of quantum chromodynamics (QCD) in the non-perturbative regime [1–3]. The topic of all-charm tetraquarks has gained significant interest recently. The LHCb Collaboration reported the first observation of a narrow resonance near 6.9 GeV ($X(6900)$) in the di- J/ψ mass spectrum in 2020 [4], interpreted as a all-charm tetraquark ($T_{cc\bar{c}\bar{c}}$) [3, 5–11]. The ATLAS and CMS experiments later confirmed the observation of $X(6900)$, as well as another broad structure around 6.6 GeV [12, 13]. Recently, CMS reported measurements of the quantum numbers of three all-charm tetraquarks, including a further resonance near 7.1 GeV, favoring a scenario of tightly bound states [14]. It becomes interesting to search for similar resonances in the $J/\psi + \psi(2S)$ spectrum and gain more insights into these exotic states. The decay $\psi(2S) \rightarrow \mu\mu$ was investigated by ATLAS in Ref. [12]. In this Letter, the decay $\psi(2S) \rightarrow J/\psi\pi^+\pi^- \rightarrow 2\mu 2\pi$ is also reconstructed, whose total branching fraction is more than twice that of the former. The analysis uses 140 fb^{-1} of proton–proton (pp) collision data collected by the ATLAS experiment at $\sqrt{s} = 13 \text{ TeV}$ during 2015–2018.

The ATLAS experiment [15] is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and nearly 4π coverage in solid angle.¹ It consists of an inner tracking detector (ID) surrounded by a thin superconducting solenoid providing a 2T axial magnetic field, sampling electromagnetic and hadronic calorimeters and a muon spectrometer (MS). The muon and tracking systems play a crucial role in reconstructing signal events. The ID covers the pseudorapidity range $|\eta| < 2.5$ and consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker. The MS surrounds the calorimeters and is based on three large superconducting air-core toroids with eight coils each. It includes a system of tracking chambers up to $|\eta| = 2.7$ and fast detectors for triggering up to $|\eta| = 2.4$. A two-level trigger system is used to select events for offline analysis [16]. A software suite [17] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment. Events are selected for analysis only if all detector systems are in good operating condition [18].

Monte Carlo (MC) simulated samples are used to study the mass resolution and signal efficiency and to estimate some of the background processes. The main backgrounds are prompt di-charmonium (J/ψ or $\psi(2S)$) production via single [19, 20] and double [21, 22] parton scattering (SPS and DPS), non-prompt charmonium production from b -hadron (via $b\bar{b}$ production) decays where the charmonium vertex is displaced from the pp collision vertex, prompt single charmonium production, and non-resonant di-muon production. The last two enter the analysis due to tracks misidentified as muons and are collectively categorized as “others”. PYTHIA 8.244 [23] was used to generate the other three backgrounds. Both the color-singlet and color-octet intermediate states were included for J/ψ and $\psi(2S)$. The signal was generated with PYTHIA 8.306 [24]. The A14 set of tuned parameters [25] and the NNPDF23LO [26] parton distribution function were used. Final-state radiation in particle decays was simulated by PHOTOS [27]. Exclusive decays of $J/\psi \rightarrow 2\mu$ and $\psi(2S) \rightarrow 2\mu$ or $\psi(2S) \rightarrow J/\psi\pi^+\pi^- \rightarrow 2\mu 2\pi$ are enforced. The decay products are evenly distributed in the final state phase space, but the ratio of signal efficiencies for the two processes depends little on this assumption, according to the MC study, which is relevant for the ratio of signal yields in different channels.

The events were collected by di-muon and tri-muon trigger paths with at least one di-muon pair whose mass is consistent with J/ψ or $\psi(2S)$ and with trigger muon p_T thresholds tuned for different data-taking periods [28]. The trigger efficiency relative to offline requirements for both signals $X(6900) \rightarrow J/\psi + \psi(2S) \rightarrow 4\mu(+2\pi)$

¹ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector and the z -axis along the beam pipe. The x -axis points from the IP to the center of the LHC ring, and the y -axis points upwards. Polar coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z -axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln \tan(\theta/2)$. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

is about 65%. Muons are reconstructed by matching tracks found in the ID and the MS. They must satisfy the *loose* identification criteria [29]. In all channels, events are required to have at least four muons with two opposite-charge pairs. In the $4\mu + 2\pi$ channel, two additional opposite-sign (OS) charged tracks fulfilling the *loose* criteria [30, 31] are required. The ID tracks of four muons (plus two pions for $4\mu + 2\pi$) are fitted to a common vertex with the mass of each charmonium constrained [32] to its world average value [33]. Requirements are imposed on quantities such as the muon momentum, vertex fit quality, and the projected transverse distances between the primary vertex [34] and the candidate vertex, as shown in Table 1. Since ΔR between the two charmonia is relatively small (large) for signal resonances (backgrounds), the signal regions (SRs) are defined with $\Delta R < 0.25$, while events with $\Delta R \geq 0.25$ belong to the fit control regions (CRs) used to validate and constrain the background normalizations. Data events in SRs were not examined until the background estimation procedure was fully defined. In the $4\mu + 2\pi$ channel, a boosted decision tree (BDT) is employed to reduce the feed-up background that is explained below.

Table 1: Event selection criteria for different analysis regions. Details can be found in App. 1.

4 μ channel		4 $\mu + 2\pi$ channel	
SR	CR	SR	CR
Di-muon or tri-muon triggers, oppositely charged muons from each charmonium, <i>Loose</i> muons, $p_{\text{T}1,2,3,4} > 4, 4, 3, 3$ GeV and $ \eta_{1,2,3,4} < 2.5$ for the four muons, $m_{J/\psi} \in [2.94, 3.25]$ GeV, $m_{\psi(2S)} \in [3.56, 3.80]$ GeV			
—		Two <i>loose</i> OS ID tracks with $p_{\text{T}} > 0.5$ GeV for pions, BDT requirement	
$\chi^2_{4\mu}/N < 3$, $ L_{xy}^{4\mu} < 0.2$ mm, $ L_{xy}^{\text{charm}} < 0.3$ mm, $m_{4\mu} < 11$ GeV		$\chi^2_{4\mu+2\pi}/N < 3$, $ L_{xy}^{4\mu+2\pi} < 0.2$ mm, $ L_{xy}^{\text{charm}} < 0.3$ mm, $m_{4\mu+2\pi} < 11$ GeV	
$\Delta R(J/\psi, \psi(2S)) < 0.25$	$\Delta R(J/\psi, \psi(2S)) \geq 0.25$	$\Delta R(J/\psi, \psi(2S)) < 0.25$	$\Delta R(J/\psi, \psi(2S)) \geq 0.25$

The backgrounds are estimated in the order of “others”, non-prompt, DPS, and SPS. The “others” background, consisting of events with at most one real charmonium, is modeled from data itself by requiring at least one charmonium candidate to contain a track that fails the muon identification. The charmonium mass sideband events are used to implement the normalization and corrections for this background. The non-prompt charmonium background is estimated with MC, which is corrected and normalized in a non-prompt CR defined by mainly reversing the L_{xy}^{charm} requirement. The SPS and DPS di-charmonium backgrounds are also estimated with MC, which have been corrected in several kinematic variables in dedicated background CRs. The SPS (DPS) CR is defined with di-charmonium mass within [8, 12] ([14, 25]) GeV, where it is relatively enriched and signal is depleted. The corrections are implemented by assigning event weights to MC events such that distributions of kinematic variables in the MC match the data in the CRs. The corrections are then applied to all regions. More details can be found in App. 2.

To combine with the di- J/ψ channel, the statistical inputs from Ref. [12] were used. This channel receives a feed-down background from the $J/\psi + \psi(2S)$ channels where there is a J/ψ in the decay products of $\psi(2S)$, such as $\psi(2S) \rightarrow J/\psi \pi^+ \pi^-$ or $J/\psi + \text{ neutrals}$, and $\psi(2S) \rightarrow \gamma \chi_{c0,1,2} \rightarrow \gamma \gamma J/\psi$. Meanwhile, the $J/\psi + \psi(2S) \rightarrow 4\mu + 2\pi$ channel receives a feed-up background from the di- J/ψ channel, where four muons are combined with two random charged tracks that are reconstructed under the pion hypothesis.

The feed-up background is reduced by about 65% with the BDT, while 92% of the signal is retained. For BDT training, the MC events containing true $\psi(2S) \rightarrow J/\psi + 2\pi$ decays that are correctly reconstructed are treated as the signal, while the ones with random pions are treated as the background. More details can be found in App. 3.

Since the kinematics and normalization are very similar between two randomly selected OS and same-sign (SS) charged tracks, the feed-up background yield in SR and CR after the BDT selection is constrained by two signal-free regions, SS SR-like and SS CR-like. These are defined by requiring two SS pions, while all other selection criteria are identical to those of Table 1. The mass shape of feed-up is obtained from MC.

Unbinned maximum likelihood fits are performed to extract the signal information from data in the 4μ and $4\mu + 2\pi$ mass spectra. The likelihood used for the fit is

$$\mathcal{L} = \mathcal{L}_{SR}(\boldsymbol{\theta}, \lambda) \cdot \mathcal{L}_{CR}(\boldsymbol{\theta}) \cdot \prod_{j=1}^K G\left(\theta'_j; \theta_j, \sigma_j\right), \quad (1)$$

where \mathcal{L}_{SR} and \mathcal{L}_{CR} are the likelihoods in the SRs and CRs, λ are the parameters of interest, θ_j are nuisance parameters (NP) accounting for systematic uncertainties shared between SRs and CRs. Each NP follows a Gaussian distribution having a subsidiary measurement θ'_j , with mean θ_j and width σ_j from pre-fit central values and uncertainties. Background yields in 4μ CR, $4\mu + 2\pi$ OS CR, and SS CR-like are used to constrain the background yields in 4μ SR, $4\mu + 2\pi$ SR, and SS SR-like, respectively, in a simultaneous fit. Each constraint is implemented as a ratio of total background yields in an SR and its corresponding CR, as predicted by pre-fit background estimations. The signal mass and width are shared in the SRs, with freely floating signal yields constrained by their ratio, as predicted by the decay branching fractions of $\psi(2S)$ and MC efficiencies. The feed-up background has the same shape and yield in $4\mu + 2\pi$ OS SR and SS SR-like. For fits that also involve the di- J/ψ channel, the corresponding likelihood from Ref. [12] is multiplied with Eq. 1.

The signal resonances can be either standalone or interfering. They can interfere with each other or interfere with the SPS background. Thus, in this Letter, three representative signal models are studied. Models A [12, 13] and B [4, 12] assume that the $X(6900)$ state observed in the di- J/ψ channel also decays into $J/\psi + \psi(2S)$. In model A, the signal probability density functions (PDF) consist of two interfering S-wave Breit–Wigner (BW) resonances, which read

$$f_{s,\text{di-}J/\psi}^A(x) = \left| \sum_{i=1}^2 \frac{z_i}{m_i^2 - x^2 - im_i\Gamma_i(x)} \right|^2 \sqrt{1 - \frac{4M_{J/\psi}^2}{x^2}} \otimes R(\boldsymbol{\theta}),$$

$$f_{s,J/\psi+\psi(2S)}^A(x) = \left| \sum_{i=1}^2 \frac{z_i}{m_i^2 - x^2 - im_i\Gamma_i(x)} \right|^2 \sqrt{1 - \left(\frac{M_{J/\psi} + M_{\psi(2S)}}{x} \right)^2} \otimes R(\boldsymbol{\theta}), \quad (2)$$

where x is the event-by-event reconstructed di-charmonium mass, m_i and $\Gamma_i(x)$ are resonance mass and width² parameters ($m_1 < m_2$), M represents the charmonium PDG mass, z_i are complex numbers representing the relative magnitudes and phases (z_1 is fixed to unity with a zero phase without loss of generality), and $R(\boldsymbol{\theta})$ is the mass resolution function convolved (\otimes) with the BWs. The function is a sum of

² For S-waves, $\Gamma_i(x) = \Gamma_i \frac{m_i}{x} \frac{q_i}{q_i}$, where q (q_i) is the momentum of one charmonium in the rest frame of the di-charmonium system at the invariant mass equal to x (m_i) [33].

three Gaussians with different widths and a common mean. Model *B* has two BWs – one interferes with SPS, while the other, $X(6900)$, remains standalone. The signal+SPS PDF in the di- J/ψ channel reads

$$f_{s+\text{SPS}, \text{di-}J/\psi}^B(x) = \left(\left| \frac{z_1}{m_1^2 - x^2 - im_1\Gamma_1(x)} + A(x)e^{i\phi_{\text{SPS}}} \right|^2 + \left| \frac{1}{m_2^2 - x^2 - im_2\Gamma_2(x)} \right|^2 \right) \sqrt{1 - \frac{4M_{J/\psi}^2}{x^2}} \otimes R(\theta), \quad (3)$$

where $A(x)$ and ϕ_{SPS} are the SPS background amplitude and phase relative to the resonance at m_1 . The term $|A(x)|^2$ reproduces the non-interfering SPS background from the MC prediction. The signal PDF in the $J/\psi + \psi(2\text{S})$ channels is similar to Eq. (2), but has only the contribution from $X(6900)$.

The signal yields of $X(6900)$ ³ in the $\text{di-}J/\psi \rightarrow 4\mu$ ($N_{\text{di-}J/\psi}$), $J/\psi + \psi(2\text{S}) \rightarrow 4\mu$ ($N_{4\mu}$) and $J/\psi + \psi(2\text{S}) \rightarrow 4\mu + 2\pi$ ($N_{4\mu+2\pi}$) channels are expressed as one yield ($N_{4\mu}$) and two ratios. The ratio $N_{4\mu}/N_{\text{di-}J/\psi}(R)$ is a function of $R = \Gamma_{X(6900) \rightarrow J/\psi + \psi(2\text{S})}/\Gamma_{X(6900) \rightarrow \text{di-}J/\psi}$ where Γ is the partial decay width. It reads

$$\frac{N_{4\mu}}{N_{\text{di-}J/\psi}} = R \cdot \frac{\mathcal{B}(\psi(2\text{S}) \rightarrow \mu\mu) \cdot \varepsilon_{4\mu}}{\mathcal{B}(J/\psi \rightarrow \mu\mu) \cdot \varepsilon_{\text{di-}J/\psi}}, \quad (4)$$

where \mathcal{B} are the charmonium decay branching fractions, $\varepsilon_{4\mu}$ and $\varepsilon_{\text{di-}J/\psi}$ are signal efficiencies for $X(6900) \rightarrow J/\psi + \psi(2\text{S}) \rightarrow 4\mu$ and $X(6900) \rightarrow \text{di-}J/\psi \rightarrow 4\mu$, respectively. This ratio at equal partial decay widths is predicted to be $N_{4\mu}/N_{\text{di-}J/\psi}(R=1) = 0.145 \pm 0.016$, and similarly, the other ratio is $N_{4\mu}/N_{4\mu+2\pi} = 0.880 \pm 0.072$, where the errors include both statistical and systematic uncertainties.

In model *C*, only $J/\psi + \psi(2\text{S})$ channels are considered in the simultaneous fit, and the signal PDF consists of a single BW function. To test the potential existence of a second resonance near 7.2 GeV ($X(7200)$) in the $J/\psi + \psi(2\text{S})$ channels, a standalone $X(7200)$ is included in each of the models described above for a new fit. The mass and width of this resonance are fixed at 7.22 GeV and 0.09 GeV, as determined in the previous ATLAS publication [12]. Evidence for this resonance was also reported by LHCb [4] and CMS [13]. The ratio of signal yields of $X(6900)$ and $X(7200)$, $r = N_{X(6900)}/N_{X(7200)}$, is treated as a free parameter in the fit. Using the CL_s method [35], an upper limit on this ratio at the 95% confidence level (CL) is derived.

Systematic uncertainties arise from signal modeling, background estimate and detector effects. Signal modelling uncertainties include variations of the signal resonance's natural decay width, turning on or off the correction on its p_T , as well as uncertainties in the charmonium decay branching fractions [33]. Detector-related uncertainties include the muon momentum calibration, trigger, reconstruction and identification efficiencies. A systematic uncertainty is assigned due to the use of mass-independent fixed-width resolution functions. Background uncertainties account for the impact of statistical fluctuations in the background MC and the correction of the di-charmonium p_T distribution on its mass shape parameters for the total backgrounds in SRs. For the SPS process, a variation of the Pythia parameter `pT0timesMPI` [23] in the range 0.61 ± 0.05 is included, which was determined in the SPS CR. In the 4μ channel, a mass shape non-closure uncertainty for “others” is also included. In the $4\mu + 2\pi$ channel, the mass shape uncertainty of the feed-up background is evaluated by varying the fitted signal parameters from the di- J/ψ channel. Systematic uncertainties also include the addition of $X(7200)$ and potential biases from the fit as determined from toy MC studies. The S-wave BW functions are replaced by P-wave or D-wave [36, 37] to test the variations of fitted parameters, which contributes the largest uncertainty for $X(6900)$'s width in model

³ For model *A*, the $X(6900)$ signal yield corresponds to its own BW function squared, without the interference with other resonances taken into account.

C. When combining with the di- J/ψ channel, the same systematic uncertainties are correlated with the $J/\psi + \psi(2S)$ channels. More details can be found in App. 2 & 4.

The fitted di- J/ψ and $J/\psi + \psi(2S)$ mass spectra for models A and B are shown in Figure 1. The fitted $J/\psi + \psi(2S)$ mass spectra using model C are shown in Figure 2. The fitted masses and widths of the resonances, and the ratio of partial widths R are given in Table 2. The signal significance of $X(6900)$ for model C with signal shape parameters fixed to their best-fit values reaches 8.9σ ⁴. Compared to Ref. [12], more precise mass and width are determined in the $J/\psi + \psi(2S)$ channels. The results of model C are consistent with those from the individual fits of the 4μ and $4\mu + 2\pi$ channels. By including $X(7200)$ in model C, r is found to be 0.12 ± 0.11 , with an upper limit of 0.41 at 95% CL, taking into account variations in the mass and width of the $X(7200)$ from Ref. [12]. The inclusion of $X(7200)$ in models A and B yields consistent results.

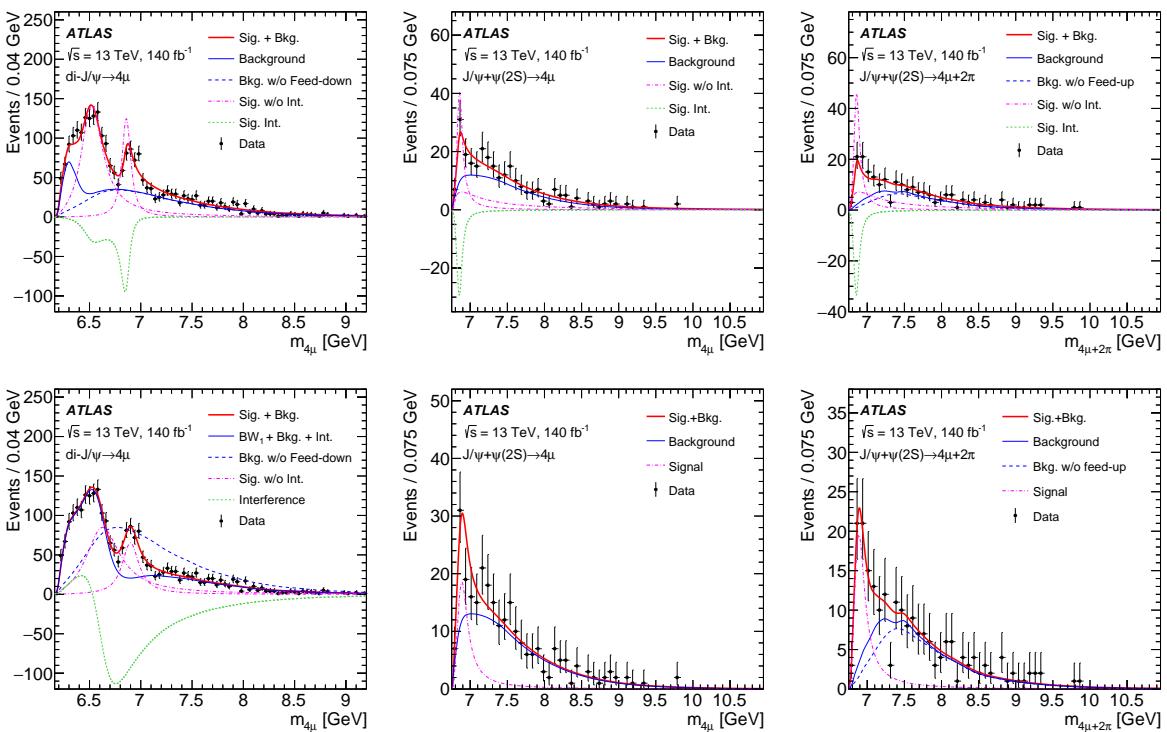


Figure 1: Fits to the di- J/ψ and $J/\psi + \psi(2S)$ mass spectra in the SRs for model A (top panel) and B (bottom panel). For each model, the di- J/ψ spectrum (left) and the $J/\psi + \psi(2S)$ spectra in the 4μ (middle) and $4\mu + 2\pi$ (right) channels are shown. The purple dash-dotted lines represent the components of individual resonances, and the green short dashed ones represent the interferences. Note that no interference is present in the $J/\psi + \psi(2S)$ channels with model B since $X(6900)$ is standalone.

In summary, to better understand the excess observed in the $J/\psi + \psi(2S)$ mass spectrum [12], both the $\psi(2S) \rightarrow \mu\mu$ and $\psi(2S) \rightarrow J/\psi + 2\pi$ decays, where the latter is new, are investigated using pp collisions data collected by the ATLAS experiment at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 140 fb^{-1} . Three different fit models are carried out. Model A (two interfering resonances) and model B

⁴ The asymptotic formula based on the profile likelihood ratio, $Z = \sqrt{2 \ln \frac{\mathcal{L}(s, \hat{\theta})}{\mathcal{L}(0, \hat{\theta})}}$, is used to calculate the overall significance, where s is the signal yield and θ are NPs [38]. In the calculations, the signal shape parameters are all fixed to their best-fit values.

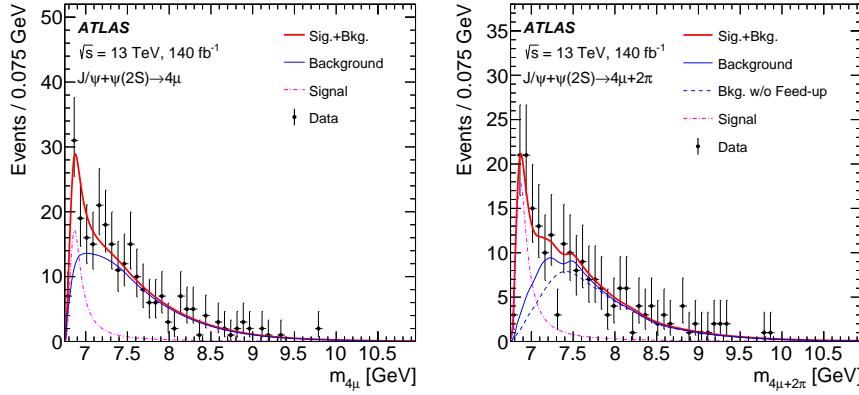


Figure 2: Fits to the $J/\psi + \psi(2S)$ mass spectra with model C in the SRs of the 4μ (left) and $4\mu + 2\pi$ (right) channels. The purple dash-dotted lines represent the signal resonances.

Table 2: The fitted masses and natural widths of $X(6900)$ with three fit models. The ratio of partial widths, $R = \Gamma_{X(6900) \rightarrow J/\psi + \psi(2S)} / \Gamma_{X(6900) \rightarrow \text{di-}J/\psi}$, is also given for model A and B . The first uncertainty is statistical, while the second one is systematic.

	model A	model B	model C
m / GeV	$6.860 \pm 0.023 \pm 0.010$	$6.902 \pm 0.008 \pm 0.010$	$6.884 \pm 0.017^{+0.058}_{-0.005}$
Γ / GeV	$0.082 \pm 0.032 \pm 0.015$	$0.183 \pm 0.025 \pm 0.007$	$0.178 \pm 0.054^{+0.176}_{-0.024}$
R	$1.08 \pm 0.20^{+0.40}_{-0.09}$	$0.93 \pm 0.17 \pm 0.11$	—

(one interfering with SPS and the other standalone) assume that the resonance $X(6900)$ decays into both the di- J/ψ and $J/\psi + \psi(2S)$ final states, while model C assumes a standalone resonance in the $J/\psi + \psi(2S)$ channels. The ratio of partial decay widths, $R = \Gamma_{X(6900) \rightarrow J/\psi + \psi(2S)} / \Gamma_{X(6900) \rightarrow \text{di-}J/\psi} = 1.08 \pm 0.20^{+0.40}_{-0.17}$, is obtained with model A being nominal and B as a systematic uncertainty. The fitted resonance mass in all three models is consistently around 6.9 GeV. The fitted width is about 0.08 GeV with model A , and about 0.18 GeV with model B and C . The mass and width of $X(6900)$ obtained in model C are consistent in the two $\psi(2S)$ decay channels. They are also consistent with, and supersede, the corresponding values of model β in Ref. [12]. The signal significance is 8.9σ for the resonance near 6.9 GeV in the $J/\psi + \psi(2S)$ channels. The existence of $X(7200)$ in the $J/\psi + \psi(2S)$ channels is tested in each model. The ratio of signal yields for $X(7200)$ to $X(6900)$ is found to be 0.12 ± 0.11 , with an upper limit of 0.41 at 95% CL. These results confirm the presence of structures in the $J/\psi + \psi(2S)$ channels, favoring a single-resonance hypothesis near 6.9 GeV, while the existence of a potential resonance near 7.2 GeV is not supported by the current data. All three models provide a reasonable description of the data, two of which indicate a ratio of the partial decay widths of $X(6900) \rightarrow J/\psi + \psi(2S)$ and $X(6900) \rightarrow 2J/\psi$ near 1. In the future, more data will allow to better determine the nature of this excess, including its true model and quantum numbers, and to investigate potential additional resonances.

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Appendix

1 Event selection

Requirements on a number of variables are imposed to suppress backgrounds and purify signals, as shown in Table 1. The meaning of variables in the table is listed below.

- $m_{J/\psi}, m_{\psi(2S)}$: The charmonium invariant mass before the vertex fit.
- $m_{4\mu}, m_{4\mu+2\pi}$: The 4μ or $4\mu + 2\pi$ vertex mass after the vertex fit.
- $\chi^2_{4\mu}/N, \chi^2_{4\mu+2\pi}/N$: The 4μ or $4\mu + 2\pi$ vertex fit quality χ^2 divided by the number of degrees of freedom N . The vertex candidate with the lowest χ^2/N is selected in events with more than one candidate meeting the criteria on χ^2/N .
- $L_{xy}^{4\mu}, L_{xy}^{4\mu+2\pi}, L_{xy}^{\text{charm}}$: The distance in the transverse plane from the primary vertex to the $4\mu, 4\mu + 2\pi$ vertices and charmonium subvertex, projected onto the direction of the vertex candidate’s transverse momentum, respectively. The charmonium subvertex is obtained by reverting the tracks from its decay with the subvertex mass constrained to the charmonium’s PDG mass. The primary vertex is the $p\bar{p}$ collision vertex. If there are multiple primary vertices in the event due to pileup [40], the one closest to the candidate vertex in z is chosen. These quantities can be negative due to the resolution effect.

2 Background estimation

While “others” is estimated in a data-driven way, the three other background sources are modelled by MC. Data events used to model “others” are obtained by applying the same requirements as in Table 1, except that there is no ΔR requirement, one of the four muons should fail *loose* criteria, the vertex quality is relaxed to $\chi^2/N < 15$ and the mass range is extended to $m_{4\mu(+2\pi)} < 25$ GeV. The CRs defined for these backgrounds are listed in Table 3.

Table 3: Requirements for background CRs. They are the same as in Table 1, except for what are listed here.

“others”	non-prompt	DPS	SPS
$m_{J/\psi} \in [2.60, 2.76]$ GeV or $m_{J/\psi} \in [3.34, 3.50]$ GeV for either J/ψ ;	$L_{xy}^{\text{charm}} > 0.3$ mm for either charmonium,	No ΔR or BDT requirements,	No ΔR or BDT requirements,
$m_{\psi(2S)} \in [3.35, 3.48]$ GeV or $m_{\psi(2S)} \in [3.88, 4.10]$ GeV for $\psi(2S)$	$\chi^2_{4\mu(+2\pi)}/N < 15$, $m_{4\mu(+2\pi)} < 25$ GeV	$m_{4\mu(+2\pi)} \in [14, 25]$ GeV	$m_{4\mu(+2\pi)} \in [8, 12]$ GeV

The “others”, non-prompt and DPS CRs are orthogonal to the analysis SRs and CRs, but the SPS CR has some overlap with them. However, the overlap only happens for $m_{4\mu(+2\pi)} > 8$ GeV where the signal is basically zero. The background CRs are used to both derive kinematic corrections and normalize the relevant background. The distributions of several kinematic variables are corrected by assigning event

weights to MC events so that their distributions are consistent with data in the background CR. The consistency between the background and data is also improved by these weights for other variables whose distributions are not directly corrected. The variables corrected are listed in Table 4. The correction weights are derived in the form of polynomial functions through several iterations. The iterations stop when the function parameters obtained in the current iteration are consistent with the previous one within their corresponding uncertainties.

Table 4: Variables that are corrected in different background CRs.

“others”	non-prompt	DPS	SPS
4^{th} muon p_{T} , charmonium p_{T} , $m_{4\mu(+2\pi)}$	4^{th} muon p_{T}	di-charmonium p_{T} , $\Delta\eta$ between charmonia, 4^{th} muon p_{T} , 2 nd pion p_{T}	di-charmonium p_{T} , $m_{4\mu(+2\pi)}$, $\Delta\eta$ and $\Delta\phi$ between charmonia, 4^{th} muon p_{T} , 2 nd pion p_{T}

As can be seen from Figure 3, the contributions of non-prompt and DPS are very small in the SR, so it is crucial to control the di-charmonium mass shape for SPS and “others” in the SR. The largest shape systematic uncertainties for SPS come from MC statistical uncertainty and the PYTHIA parameter pT0timesMPI. The latter is varied to form different MC templates, and the background is compared with data in the SPS CR, in which way its nominal value and 1σ uncertainty are obtained. The SPS mass shape is also validated in the analysis CRs as shown in Figure 3, especially in the region near the threshold. In the $J/\psi + \psi(2\text{S}) \rightarrow 4\mu$ channel, “others” is also important due to the smaller signal purity under $\psi(2\text{S})$ than J/ψ . Its modeling is checked in the non-prompt region as defined in Table 3, since “others” in this region is dominant and the non-prompt is actually very small. Any mass shape difference between background and data is attributed to the “non-closure” systematic uncertainty. The di-charmonium mass distributions in the total background CR (similar to SPS and DPS CRs but with $m_{4\mu(+2\pi)} \in [8, 25]$ GeV), analysis CR and SR are shown in Figure 3. Because the signal and background cross-sections are not measured in this analysis (which would involve many theoretical assumptions), their yields and efficiencies are not provided. Instead, the pre-fit fractions of four different backgrounds in the SRs are listed in Table 5.

Table 5: Prefit fractions of four different backgrounds in the SRs.

Channel	“others”	non-prompt	DPS	SPS
4μ	47%	0.8%	2.5%	49%
$4\mu + 2\pi$	14%	1.4%	3.6%	82%

3 Feed-up background BDT variables and distributions

In the $4\mu + 2\pi$ channel, a BDT with gradient boost [41] is used to suppress backgrounds where the pions are not from real $\psi(2\text{S})$ decays. Input variables to the BDT include χ^2/N of the $\psi(2\text{S})$ subvertex, the invariant mass of the two pions ($m_{\pi\pi}$), the cosine of the angle between the J/ψ direction in the $\psi(2\text{S})$ rest frame and the $\psi(2\text{S})$ direction in the lab frame ($\cos\theta_X$), and the scalar sum of two pions’ transverse momenta

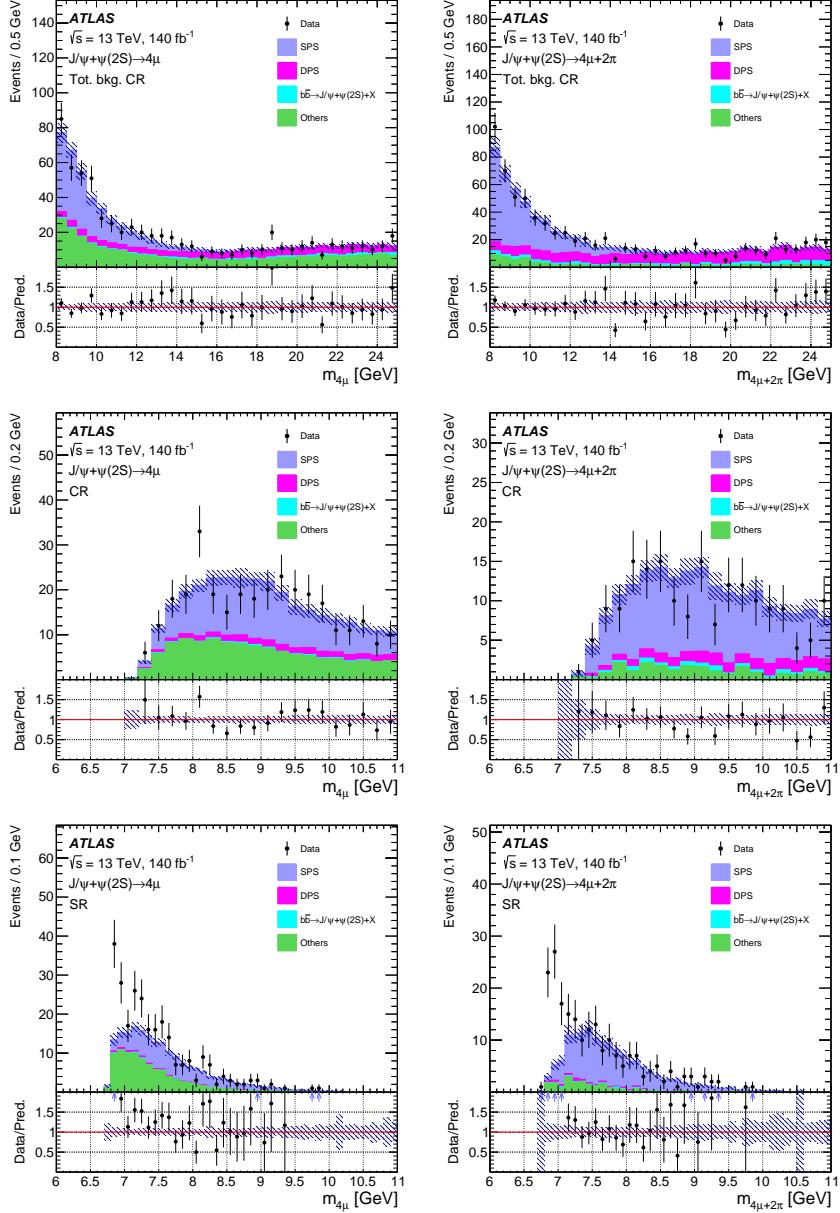


Figure 3: The $J/\psi + \psi(2S)$ mass spectra in the total background CR (top), analysis CR (middle) and SR (bottom) of the 4μ (left) and $4\mu + 2\pi$ (right) channels before the fit (excess in SR is due to the signal). $b\bar{b} \rightarrow \text{charmonia} + X$ represents the non-prompt background. The bars (shaded areas) represent uncertainties of data (background predictions) in each bin. The arrows in the lower panel indicate that the ratio of data to background prediction is out of range in that bin.

$(\sum p_T^\pi)$. Because pions from $\psi(2S)$ decay follow a phase space distribution in the MC, the $m_{\pi\pi}$ spectrum is reweighted according to the Voloshin-Zakharov model [42], and the nominal and 1σ uncertainty of the model parameter λ are taken from Ref. [43]. Distributions of these input variables, and the BDT scores, in the total background CR are shown in Figure 4. Events with $\psi(2S)$ candidates containing random pions (such as SS pions) have low BDT scores. The score is required to be greater than -0.3 in the SR. The separation power [41] of the input variables is listed in Table 6, where higher values mean better ability to classify signal and background events.

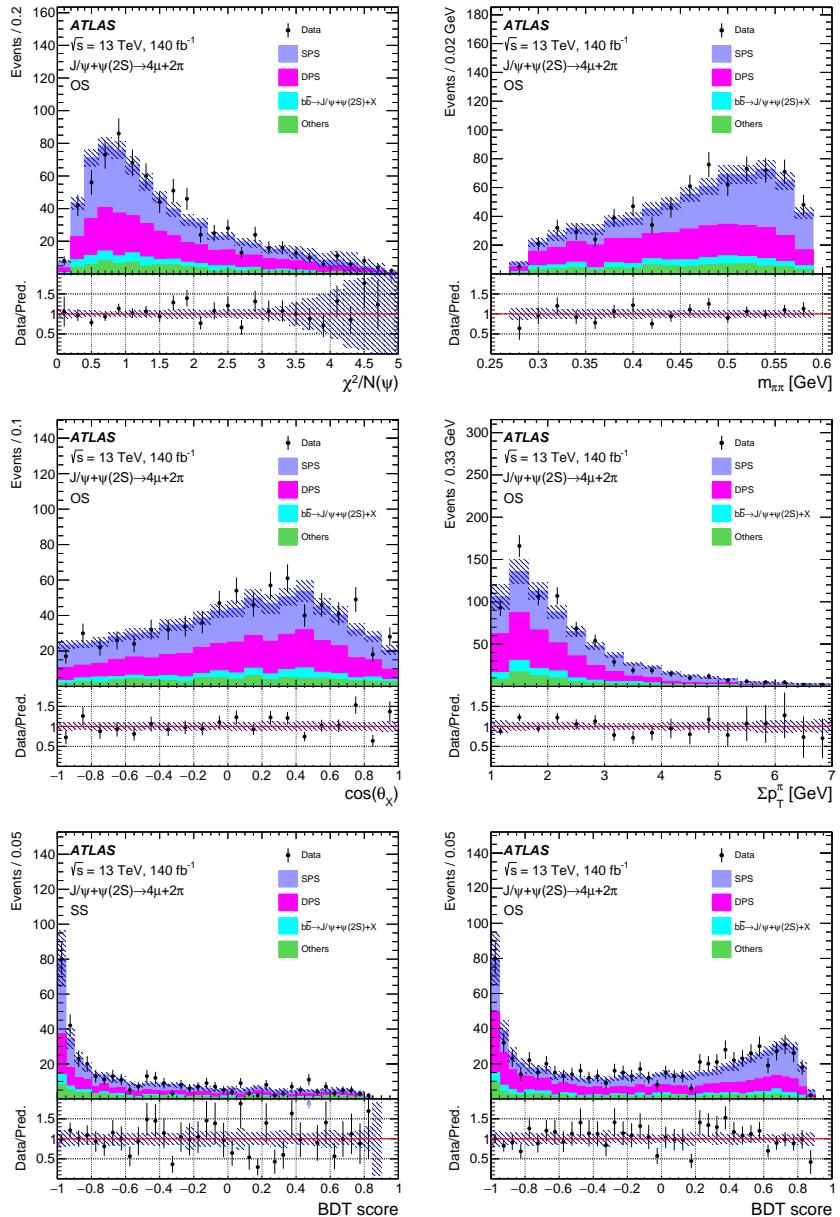


Figure 4: The distributions of input variables (top and middle) and the BDT scores for SS (bottom left) and OS (bottom right) events in the total background CR of the $4\mu + 2\pi$ channel. $b\bar{b} \rightarrow \text{charmonia} + X$ represents the non-prompt background. The bars (shaded areas) represent uncertainties of data (background predictions) in each bin. The arrows in the lower panel indicate that the ratio of data to background prediction is out of range in that bin.

Table 6: The separation power of the four input variables for BDT.

$m_{\pi\pi}$	$\sum p_T^\pi$	$\cos \theta_X$	χ^2/N of $\psi(2S)$
0.252	0.178	0.106	0.097

4 Additional figures and tables

There are three fit regions for $J/\psi + \psi(2S)$ alone: one for the $J/\psi + \psi(2S) \rightarrow 4\mu$ channel, and two (OS and SS pions) for $J/\psi + \psi(2S) \rightarrow 4\mu + 2\pi$. The SS $4\mu + 2\pi$ region is used to constrain the normalization of the feed-up background from the di- J/ψ channel, since the SS and OS feed-up yields are the same according to MC predictions. The di- J/ψ channel will contribute an additional fit region when it is combined with the $J/\psi + \psi(2S)$ channels. Common parameters such as those for the signal or the same systematic source are simultaneously determined from fits in all regions. The prefit di-charmonium mass spectrum and the simultaneous fit result with model C in the SS SR-like with $\Delta R < 0.25$ are shown in Figure 5. Fit results with the other two models in this region are very similar to Figure 5, and thus are not shown here any more.

The breakdown of uncertainties for the parameters of $X(6900)$ with three different models is given in Table 7. Only models A and B involve the near-threshold resonance around 6.5-6.6 GeV in the fit. The fitted mass and natural width of this resonance are given in Table 8.

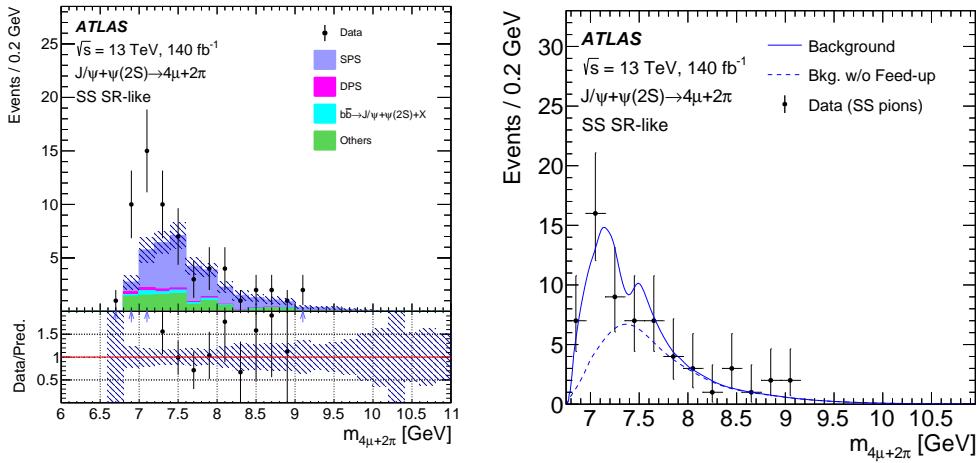


Figure 5: The $J/\psi + \psi(2S)$ mass spectrum (left) and the simultaneous fit result with model C (right) in the SS SR-like of the $4\mu + 2\pi$ channel. In the left figure, the excess in data over the total background is due to feed-up.

Table 7: Different sources of uncertainties in the mass and natural width (in MeV) of $X(6900)$, and the ratio of partial decay widths ($R = \Gamma_{X(6900) \rightarrow J/\psi + \psi(2S)} / \Gamma_{X(6900) \rightarrow \text{di-}J/\psi}$) for three different fit models.

Sources	Model A			Model B			Model C	
	m	Γ	R	m	Γ	R	m	Γ
Statistical uncertainties	± 23	± 32	± 0.20	± 8.1	± 25	± 0.17	± 17	± 54
Di- J/ψ bkg. modeling	± 5.4	± 7.7	± 0.041	± 1.4	—	—	—	—
$J/\psi + \psi(2S)$ bkg. modeling	± 4.1	± 6.7	± 0.038	—	—	—	± 2.6	± 8.6
Signal ratios	—	—	± 0.069	—	—	± 0.054	—	—
Mass resolution	± 6.8	± 8.6	± 0.033	± 1.3	± 2.2	± 0.002	± 0.3	± 4.4
Feed-up bkg.	—	—	± 0.002	—	—	± 0.002	± 0.3	± 0.6
P or D-wave BW	± 3.2	± 5.4	± 0.39	± 9.9	± 2.9	± 0.094	$+58$	$+170$
Fit bias	± 0.2	± 2.1	± 0.007	± 0.2	± 4.7	± 0.010	± 0.4	± 11
Inclusion of $X(7200)$	± 1.0	± 1.2	—	± 0.1	± 3.8	± 0.001	± 4.2	± 19

Table 8: The fitted masses and natural widths of the near-threshold resonance in the di- J/ψ channel with models *A* and *B*. The first uncertainty is statistical, while the second one is systematic.

	model A	model B
m / GeV	$6.531 \pm 0.011 \pm 0.002$	$6.646 \pm 0.018 \pm 0.021$
Γ / GeV	$0.244 \pm 0.021 \pm 0.021$	$0.390 \pm 0.045 \pm 0.037$

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