Letter

Production and polarization of *S*-wave quarkonia in potential nonrelativistic QCD

Nora Brambilla,[1,2,3] Hee Sok Chung,[1,4,*] Antonio Vairo,[1] and Xiang-Peng Wang[1]

[1]*Physik Department, Technische Universität München, James-Franck-Strasse 1, 85748 Garching, Germany*
[2]*Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2 a, 85748 Garching, Germany*
[3]*Munich Data Science Institute, Technische Universität München, Walther-von-Dyck-Strasse 10, 85748 Garching, Germany*
[4]*Excellence Cluster ORIGINS, Boltzmannstrasse 2, 85748 Garching, Germany*

(Received 22 March 2022; accepted 9 June 2022; published 23 June 2022)

Based on the potential nonrelativistic QCD formalism, we compute the nonrelativistic QCD long-distance matrix elements (LDMEs) for inclusive production of *S*-wave heavy quarkonia. This greatly reduces the number of nonperturbative unknowns and brings in a substantial enhancement in the predictive power of the nonrelativistic QCD factorization formalism. We obtain improved determinations of the LDMEs and find cross sections and polarizations of J/ψ, $\psi(2S)$, and excited Υ states that agree well with LHC data. Our results may have important implications in pinning down the heavy quarkonium production mechanism.

DOI: 10.1103/PhysRevD.105.L111503

Production of heavy quarkonia in high energy collisions provide a unique opportunity to probe the interplay between perturbative and nonperturbative aspects of QCD, as well as the hot and dense phase of QCD [1–4]. Especially, inclusive production rates of *S*-wave heavy quarkonia such as J/ψ, $\psi(2S)$, and Υ have been studied extensively in collider experiments such as the RHIC, Tevatron, *B* factories, HERA, and the LHC, and will continue to be an important subject in future colliders including the Electron-Ion Collider.

Phenomenological studies of heavy quarkonium production have mostly been carried out in the context of nonrelativistic effective field theories, which make use of the hierarchy of energy scales $m \gg mv \gg mv^2$ associated with a heavy quarkonium state. Here, m is the heavy quark mass, and v is the velocity of a heavy quark in the heavy quarkonium rest frame. Nonrelativistic QCD (NRQCD) follows from integrating out the scale of the heavy quark mass m [5,6]. NRQCD provides a factorization formalism that describes the inclusive cross section of a heavy quarkonium in terms of sums of products of perturbatively calculable short-distance coefficients (SDCs) and nonperturbative long-distance matrix elements (LDMEs). The LDMEs have known scalings in v, so that in practice the factorization formula is truncated at a desired accuracy in v. NRQCD factorization for inclusive production is expected to be accurate up to relative order m^2/p_T^2 in the expansion in powers of m^2/p_T^2, where p_T is the transverse momentum of the quarkonium produced in the collision [6–10]. Hence, large-p_T cross sections of heavy quarkonia are described by the NRQCD factorization formalism in terms of a limited number of LDMEs, which depend only on the nonperturbative nature of the heavy quarkonium state but are process independent.

For decades a huge effort has been put into computing the SDCs and determining the LDMEs. As it has not been known how to compute the LDMEs from first principles, the determinations of the LDMEs have mostly relied on measured cross section data. This approach has led to inconsistent sets of LDMEs that give contradicting predictions, depending on the choice of data and the organization of the QCD perturbation series [11–21]. Also the signs of the LDMEs can differ between different determinations. As none of the existing determinations are able to give a comprehensive description of important observables, it is fair to say that the production mechanism of heavy quarkonium still remains elusive [22].

Recently, a formalism for computing the production LDMEs has been developed in Refs. [23,24] based on the effective field theory potential NRQCD (pNRQCD), which is obtained by integrating out the scale of order mv [25–27]. The pNRQCD formalism provides expressions for

[*]Present address: Department of Physics, Korea University, Seoul 02841, Korea.

the LDMEs in terms of quarkonium wave functions at the origin, which can be computed by solving the Schrödinger equation, and gluonic correlators, which are universal quantities that do not depend on the specific heavy quarkonium state and can in principle be computed in lattice QCD. This results in a reduction of the number of nonperturbative unknowns which greatly enhances the predictive power of NRQCD factorization. The pNRQCD formalism has been successfully applied to the production of P-wave heavy quarkonia, and the phenomenological results agree well with available measurements at the LHC [23,24]. It has been anticipated that the application of the pNRQCD formalism to production of S-wave heavy quarkonia may help scrutinize the LDMEs and the applicability of the NRQCD factorization formalism.

In this work we compute, for the first time, the NRQCD LDMEs for production of S-wave heavy quarkonia in the pNRQCD formalism. We work in the strongly coupled regime, $v \gtrsim \Lambda_{\rm QCD}/m$, which we assume to be appropriate for J/ψ, $\psi(2S)$, and excited Υ states. Based on the results for the LDMEs that we obtain, we compute production rates of S-wave quarkonia at the LHC and compare them with data.

The inclusive cross section of a spin-1 S-wave heavy quarkonium V is given in the NRQCD factorization formalism at relative order v^4 accuracy by

$$\sigma_{V+X} = \hat{\sigma}_{^3S_1^{[1]}} \langle \mathcal{O}^V(^3S_1^{[1]})\rangle + \hat{\sigma}_{^3S_1^{[8]}} \langle \mathcal{O}^V(^3S_1^{[8]})\rangle + \hat{\sigma}_{^1S_0^{[8]}} \langle \mathcal{O}^V(^1S_0^{[8]})\rangle + \hat{\sigma}_{^3P_J^{[8]}} \langle \mathcal{O}^V(^3P_0^{[8]})\rangle. \quad (1)$$

Here, the $\hat{\sigma}_N$ are the SDCs, which correspond to the production rate of a heavy quark Q and antiquark $\bar{Q}$ in the color and angular momentum state N. The SDC $\hat{\sigma}_{^3P_J^{[8]}}$ includes contributions from $J = 0$, 1, and 2. We use spectroscopic notation for the angular momentum state of the $Q\bar{Q}$, while the superscripts [1] and [8] denote the color state of the $Q\bar{Q}$: color singlet (CS) and color octet (CO), respectively. The LDMEs are defined by [6–9]

$$\langle \mathcal{O}^V(^3S_1^{[1]})\rangle = \langle \Omega | \chi^\dagger \sigma^i \psi \mathcal{P}_{V(\boldsymbol{P}=\boldsymbol{0})} \psi^\dagger \sigma^i \chi | \Omega \rangle, \quad (2a)$$

$$\langle \mathcal{O}^V(^3S_1^{[8]})\rangle = \langle \Omega | \chi^\dagger \sigma^i T^a \psi \Phi_\ell^{\dagger ab} \mathcal{P}_{V(\boldsymbol{P}=\boldsymbol{0})} \Phi_\ell^{bc} \psi^\dagger \sigma^i T^c \chi | \Omega \rangle, \quad (2b)$$

$$\langle \mathcal{O}^V(^1S_0^{[8]})\rangle = \langle \Omega | \chi^\dagger T^a \psi \Phi_\ell^{\dagger ab} \mathcal{P}_{V(\boldsymbol{P}=\boldsymbol{0})} \Phi_\ell^{bc} \psi^\dagger T^c \chi | \Omega \rangle, \quad (2c)$$

$$\langle \mathcal{O}^V(^3P_0^{[8]})\rangle = \frac{1}{3} \langle \Omega | \chi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\boldsymbol{D}} \cdot \boldsymbol{\sigma} \right) T^a \psi \Phi_\ell^{\dagger ab} \mathcal{P}_{V(\boldsymbol{P}=\boldsymbol{0})} \times \Phi_\ell^{bc} \psi^\dagger \left(-\frac{i}{2} \overleftrightarrow{\boldsymbol{D}} \cdot \boldsymbol{\sigma} \right) T^c \chi | \Omega \rangle, \quad (2d)$$

where $|\Omega\rangle$ is the QCD vacuum, T^a are SU(3) generators, σ^i are Pauli matrices, and ψ and χ are Pauli spinors that annihilate and create a heavy quark and antiquark, respectively. The covariant derivative $\overleftrightarrow{\boldsymbol{D}}$ is defined by $\chi^\dagger \overleftrightarrow{\boldsymbol{D}} \psi = \chi^\dagger \boldsymbol{D} \psi - (\boldsymbol{D}\chi)^\dagger \psi$, with $\boldsymbol{D} = \boldsymbol{\nabla} - ig\boldsymbol{A}$, and $\boldsymbol{A}$ is the gluon field. The operator $\mathcal{P}_{\mathcal{Q}(\boldsymbol{P})}$ projects onto a state consisting of a quarkonium $\mathcal{Q}$ with momentum $\boldsymbol{P}$. The path-ordered Wilson line along the spacetime direction ℓ, defined by $\Phi_\ell = \mathcal{P} \exp[-ig \int_0^\infty d\lambda \ell \cdot A^{\rm adj}(\ell\lambda)]$, where $A^{\rm adj}$ is the gluon field in the adjoint representation, ensures the gauge invariance of the CO LDMEs [7–9]. The direction ℓ is arbitrary.

In existing studies of S-wave heavy quarkonium production, the CO LDMEs are determined by comparing Eq. (1) to cross section data. One major difficulty in this approach is that in existing studies based on hadroproduction, only certain linear combinations of the CO LDMEs are strongly constrained, while individual LDMEs are often poorly determined.

Now we compute the LDMEs in Eqs. (2) in pNRQCD using the formalism developed in Refs. [23,24]. We work at leading nonvanishing order in the quantum-mechanical perturbation theory (QMPT), where we expand in powers of v^2 and $\Lambda_{\rm QCD}/m$.

For the CS LDME $\langle \mathcal{O}^V(^3S_1^{[1]})\rangle$, we obtain at leading order in QMPT

$$\langle \mathcal{O}^V(^3S_1^{[1]})\rangle = 2N_c \times \frac{3|R_V^{(0)}(0)|^2}{4\pi}, \quad (3)$$

where $R_V^{(0)}(r)$ is the radial wave function of the quarkonium V at leading order in v. This reproduces the result obtained in the vacuum-saturation approximation in Ref. [6].

The expressions for the CO LDMEs are given by

$$\langle \mathcal{O}^V(^3S_1^{[8]})\rangle = \frac{1}{2N_c m^2} \frac{3|R_V^{(0)}(0)|^2}{4\pi} \mathcal{E}_{10;10}, \quad (4a)$$

$$\langle \mathcal{O}^V(^1S_0^{[8]})\rangle = \frac{1}{6N_c m^2} \frac{3|R_V^{(0)}(0)|^2}{4\pi} c_F^2 \mathcal{B}_{00}, \quad (4b)$$

$$\langle \mathcal{O}^V(^3P_0^{[8]})\rangle = \frac{1}{18N_c} \frac{3|R_V^{(0)}(0)|^2}{4\pi} \mathcal{E}_{00}, \quad (4c)$$

where c_F is given in Refs. [28–30] in the $\overline{\rm MS}$ scheme at the scale Λ by $c_F = 1 + \frac{\alpha_s}{2\pi}[C_F + C_A(1 + \log \Lambda/m)] + O(\alpha_s^2)$, with $C_F = (N_c^2 - 1)/(2N_c)$ and $C_A = N_c$; $\mathcal{E}_{10;10}$, $\mathcal{B}_{00}$, and $\mathcal{E}_{00}$ are gluonic correlators of dimension 2 defined by

$$\mathcal{E}_{10;10} = \left| d^{dac} \int_0^\infty dt_1 t_1 \int_{t_1}^\infty dt_2 g E^{b,i}(t_2) \times \Phi_0^{bc}(t_1;t_2) g E^{a,i}(t_1) \Phi_0^{df}(0;t_1) \Phi_\ell^{ef} |\Omega\rangle \right|^2, \quad (5a)$$

$$\mathcal{B}_{00} = \left| \int_0^\infty dt g B^{a,i}(t) \Phi_0^{ac}(0;t) \Phi_\ell^{bc} |\Omega\rangle \right|^2, \quad (5b)$$

$$\mathcal{E}_{00} = \left| \int_0^\infty dt g E^{a,i}(t) \Phi_0^{ac}(0;t) \Phi_\ell^{bc} |\Omega\rangle \right|^2, \quad (5c)$$

where $d^{abc} = 2\,\mathrm{tr}(\{T^a, T^b\} T^c)$, $E^{a,i}(t)$, and $B^{a,i}(t)$ are chromoelectric and chromomagnetic field components, respectively, computed at the time t and space coordinate $\mathbf{0}$, and $\Phi_0(t,t') = \mathcal{P}\exp[-ig\int_t^{t'} d\tau A_0^{\mathrm{adj}}(\tau,\mathbf{0})]$ is a Schwinger line. The chromoelectric and chromomagnetic fields in the expressions for $\mathcal{E}_{10;10}$ and $\mathcal{B}_{00}$ come from the $\boldsymbol{D}^2$ and $\boldsymbol{\sigma}\cdot g\boldsymbol{B}$ terms in the NRQCD Lagrangian, respectively, while the chromoelectric fields in $\mathcal{E}_{00}$ come from the $\overleftrightarrow{\boldsymbol{D}}$ in the definition of $\langle \mathcal{O}^V(^3P_0^{[8]})\rangle$. Note that the correlators $\mathcal{E}_{10;10}$, $\mathcal{B}_{00}$, and $\mathcal{E}_{00}$ are purely gluonic quantities that do not depend on the heavy quark flavor. The expressions in Eqs. (4) are accurate up to corrections of relative order v^2 and $1/N_c^2$ [23,24].

We find the one-loop evolution equation for $\mathcal{E}_{10;10}$ given by

$$\frac{d}{d\log\Lambda}\mathcal{E}_{10;10} = \mathcal{E}_{00} \times \frac{2\alpha_s}{3\pi}\frac{N_c^2-4}{N_c} + O(\alpha_s^2). \quad (6)$$

This reproduces the known scale dependence of $\langle \mathcal{O}^V(^3S_1^{[8]})\rangle$, which cancels the explicit $\log\Lambda$ that appears in $\hat{\sigma}_{^3P_J^{[8]}}$ [6,31]. The correlator $\mathcal{B}_{00}$ also depends on the scale in a way that $c_F^2\mathcal{B}_{00}$ is scale independent at one-loop level.

We note that our results in Eqs. (4) are valid in dimensional regularization (DR), because in computing the LDMEs we have discarded scaleless power divergences which vanish in DR [24,32]. Since the correlators in Eqs. (5) contain power UV divergences which are automatically subtracted in DR, they may not be positive definite, even though they are defined as norms of states that are obtained by applying gluonic operators on the QCD vacuum.

The three correlators in Eqs. (5) and $|R_V^{(0)}(0)|$ completely fix all LDMEs that appear in Eq. (1). Since lattice determinations of the correlators are not available yet, we determine the correlators by comparing Eq. (1) to measured cross section data at the LHC. We employ the measured data for prompt J/ψ and $\psi(2S)$ production rates in Refs. [33,34] and inclusive $\Upsilon(2S)$ and $\Upsilon(3S)$ cross sections in Ref. [35]. We use p_T cuts to prevent factorization-breaking effects at small p_T from affecting the fit. In order to explore the dependence on the p_T cut, we consider two regions $p_T/(2m) > 5$ and $p_T/(2m) > 3$.

In computing the cross sections from Eqs. (1) and (4), we use the values $|R_{J/\psi}^{(0)}(0)|^2 = 0.825$ GeV^3, $|R_{\psi(2S)}^{(0)}(0)|^2 = 0.492$ GeV^3, $|R_{\Upsilon(2S)}^{(0)}(0)|^2 = 3.46$ GeV^3, and $|R_{\Upsilon(3S)}^{(0)}(0)|^2 = 2.67$ GeV^3, which we obtain by comparing the measured leptonic decay rates in Ref. [36] with the pNRQCD expressions at leading order in v and at next-to-leading order (NLO) in α_s [37]. We compute the SDCs in Eq. (1) at NLO in α_s by using the FDCHQHP package [38]. We use $m = 1.5$ GeV for charm and 4.75 GeV for bottom, and set $\Lambda = m$ for the $\overline{\mathrm{MS}}$ scale of the NRQCD LDMEs. We consider the runnings of the correlators by using the renormalization-group improved formulas at one loop; the effect of the running of $\mathcal{B}_{00}$ is numerically small, while the running of $\mathcal{E}_{10;10}$ depends on the value of $\mathcal{E}_{00}$. We consider feeddowns from P-wave quarkonia by using the measurements in Refs. [39,40], and take into account the decays of $\psi(2S)$ into J/ψ and $\Upsilon(3S)$ into $\Upsilon(2S)$ using the measured branching ratios in Ref. [41]. We take the uncertainties in the theoretical expressions for the charmonium and bottomonium cross sections to be 30% and 10% of the central values, respectively, which account for uncalculated corrections of higher orders in v^2. We neglect uncertainties from corrections of order $1/N_c^2$ and variations of scales because they are small compared to the uncertainties that we consider.

The pNRQCD results for the LDMEs imply that the ratio of the large-p_T direct production rates of $\psi(2S)$ and J/ψ is simply given by $|R_{\psi(2S)}^{(0)}(0)|^2/|R_{J/\psi}^{(0)}(0)|^2$, up to corrections of order v^2, independently of the values of the correlators. If we take into account the feeddown contributions from decays of χ_c and $\psi(2S)$ into J/ψ, we obtain $(B_{\psi(2S)\to\mu^+\mu^-} \times \sigma_{\psi(2S)+X})/(B_{J/\psi\to\mu^+\mu^-} \times \sigma_{J/\psi+X}) \approx 0.04$, which agrees well with the measured values in Ref. [33] at large p_T. Similarly, the ratio of the large-p_T direct production rates of $\Upsilon(3S)$ and $\Upsilon(2S)$ is given by $|R_{\Upsilon(3S)}^{(0)}(0)|^2/|R_{\Upsilon(2S)}^{(0)}(0)|^2$, up to corrections of order v^2. If we take into account the feeddowns from decays of $\chi_b(3P)$ into $\Upsilon(3S)$, as well as $\chi_b(3P)$, $\chi_b(2P)$, and $\Upsilon(3S)$ into $\Upsilon(2S)$, we obtain $(B_{\Upsilon(3S)\to\mu^+\mu^-} \times \sigma_{\Upsilon(3S)+X})/(B_{\Upsilon(2S)\to\mu^+\mu^-} \times \sigma_{\Upsilon(2S)+X}) \approx 0.8$, which is in fair agreement with measurements in Ref. [35].

The values of the correlators that are determined from our fits are listed in Table I. The results from the two p_T regions are consistent within uncertainties. The qualities of

TABLE I. Fit results for the correlators $\mathcal{E}_{10;10}$, $c_F^2\mathcal{B}_{00}$, and $\mathcal{E}_{00}$ for the two p_T regions in the $\overline{\mathrm{MS}}$ scheme at the scale $\Lambda = 1.5$ GeV. The SDC c_F is computed for the charm quark mass $m = 1.5$ GeV.

p_T region	$\mathcal{E}_{10;10}$ (GeV^2)	$c_F^2\mathcal{B}_{00}$ (GeV^2)	$\mathcal{E}_{00}$ (GeV^2)
$p_T/(2m) > 5$	0.860 ± 0.277	-2.25 ± 7.06	13.4 ± 4.6
$p_T/(2m) > 3$	1.17 ± 0.13	-9.79 ± 3.08	18.5 ± 2.1

TABLE II. Numerical results for the J/ψ CO LDMEs in units of 10^{-2} GeV^3. The uncertainties come from the correlators $\mathcal{E}_{10;10}$, $c_F^2\mathcal{B}_{00}$, and $\mathcal{E}_{00}$.

p_T region	$\langle\mathcal{O}^{J/\psi}(^3S_1^{[8]})\rangle$	$\langle\mathcal{O}^{J/\psi}(^1S_0^{[8]})\rangle$	$\langle\mathcal{O}^{J/\psi}(^3P_0^{[8]})\rangle/m^2$
$p_T/(2m) > 5$	1.25 ± 0.40	-1.10 ± 3.43	2.18 ± 0.75
$p_T/(2m) > 3$	1.70 ± 0.18	-4.76 ± 1.50	3.00 ± 0.34

the fits are good; we obtain $\chi^2_{\rm min}/{\rm d.o.f.} = 6.30/41$ and $14.0/71$ for $p_T/(2m) > 5$ and $p_T/(2m) > 3$, respectively. As a representative example, we show the numerical results for the J/ψ CO LDMEs in Table II. The uncertainties shown in Table I are correlated; the correlation matrix of the uncertainties in $\mathcal{E}_{10;10}$, $c_F^2\mathcal{B}_{00}$, and $\mathcal{E}_{00}$ for each p_T region is given by

$$C_{\frac{p_T}{2m}>5} = \begin{pmatrix} 0.0766 & -1.75 & 1.27 \\ -1.75 & 49.8 & -28.5 \\ 1.27 & -28.5 & 21.3 \end{pmatrix} \text{GeV}^4, \qquad (7a)$$

$$C_{\frac{p_T}{2m}>3} = \begin{pmatrix} 0.0160 & -0.348 & 0.267 \\ -0.348 & 9.49 & -5.62 \\ 0.267 & -5.62 & 4.48 \end{pmatrix} \text{GeV}^4. \qquad (7b)$$

When computing observables, we take into account these correlations in order to reduce the theoretical uncertainties. We note that the eigenvectors of the correlation matrix are almost independent of the p_T cut.

Our fits strongly constrain the value of $\mathcal{E}_{00}$ to be positive. This happens because, the ratios of the charmonium and bottomonium cross sections at comparable values of p_T/m depend mainly on the ratios of $|R_V^{(0)}(0)|^2$, the quark mass, and the running of the correlators. Since the running of $\mathcal{E}_{10;10}$ depends on $\mathcal{E}_{00}$, the pNRQCD analysis determines rather precisely $\mathcal{E}_{00}$, and eventually the CO LDME $\langle\mathcal{O}^V(^3P_0^{[8]})\rangle$ as well. This distinguishes the pNRQCD analysis from other existing approaches. A positive $\mathcal{E}_{00}$ implies that the value of $\mathcal{E}_{10;10}$ at the scale $\Lambda = m$ is larger for bottomonium than for charmonium. We expect that the sign of $\mathcal{E}_{00}$ will not change because of corrections of higher orders in α_s, as radiative corrections shall affect the charmonium and bottomonium SDCs in a similar way.

In Fig. 1 we show our results for the prompt production rates of J/ψ and $\psi(2S)$, and inclusive cross sections of $\Upsilon(2S)$ and $\Upsilon(3S)$ at the LHC center of mass energy $\sqrt{s} = 7$ TeV compared with CMS and ATLAS measurements from Refs. [33–35], which are used in our fits. The theoretical uncertainties are determined so that they encompass the uncertainties in the correlators in the two p_T regions. The pNRQCD results for the cross sections are in fair agreement with measurements at large p_T. In Fig. 1 we also show, as dotted outlined bands, the pNRQCD results where the production rates for each quarkonium state are

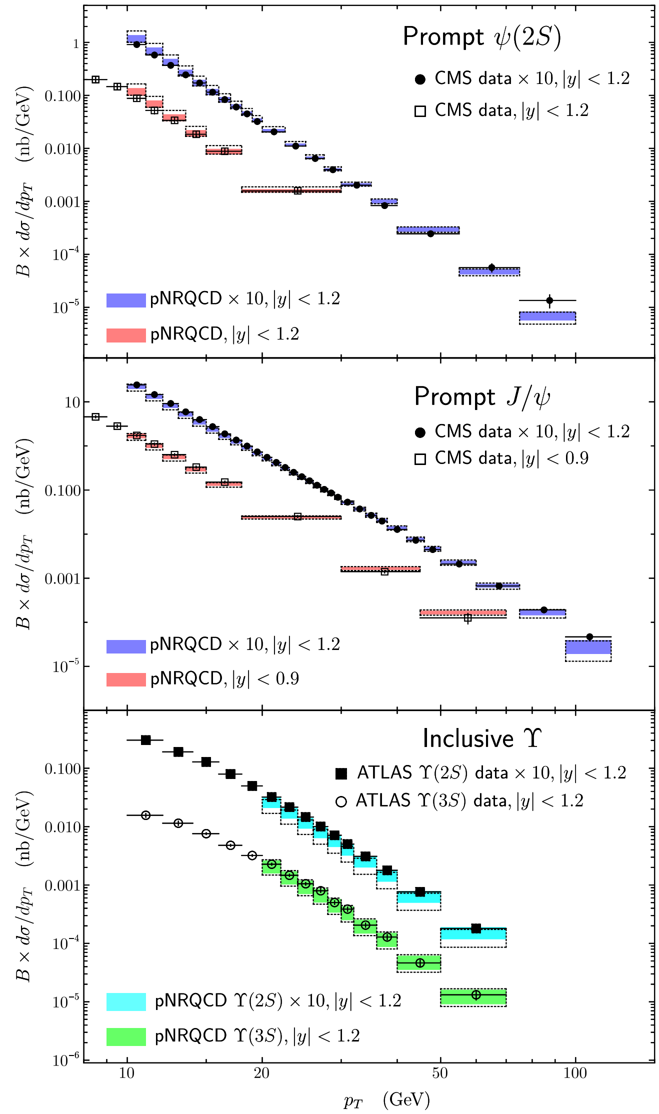

FIG. 1. The p_T-differential cross sections for J/ψ, $\psi(2S)$, $\Upsilon(2S)$, and $\Upsilon(3S)$ at the LHC center of mass energy $\sqrt{s} = 7$ TeV compared with the CMS and ATLAS measurements [33–35]. Here, B is the dilepton branching ratio. For each quarkonium state, the dotted outlined bands are pNRQCD results obtained by excluding that quarkonium data from the fit.

obtained by excluding that quarkonium data from the fit. In all cases, the results are consistent with the fits from all available data.

We note that the bulk of the cross section comes from the remnant of the cancellation between the $^3P_J^{[8]}$ and $^3S_1^{[8]}$ channels ($\hat\sigma_{^3P_J^{[8]}}$ is negative at large p_T, while $\hat\sigma_{^3S_1^{[8]}}$ is positive); moreover, the contribution from the $^1S_0^{[8]}$ channel is small. We have tested the stability of our results against the large cancellations between channels by imposing an upper p_T cut, and found that it has negligible effects to our fits.

An important observable that lets us put the CO contributions to the test is the polarization of the quarkonium at

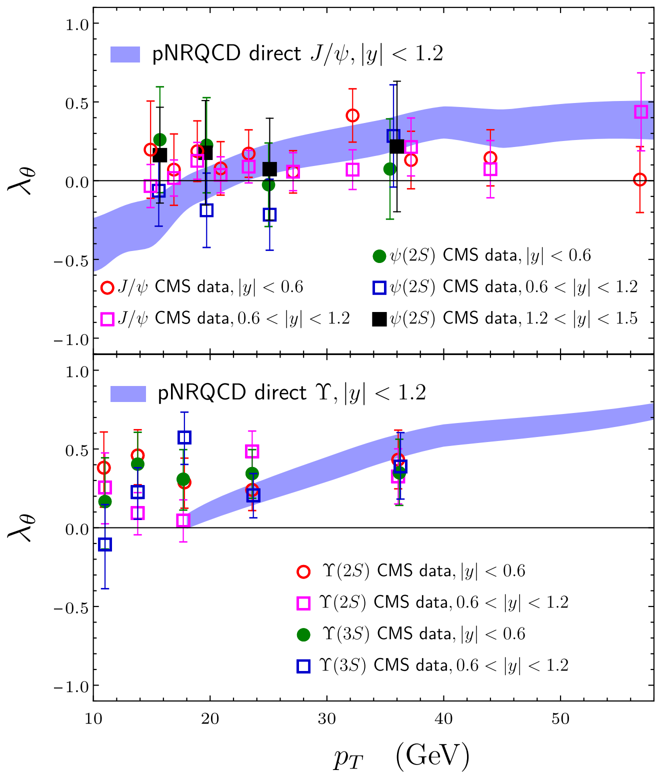

FIG. 2. The polarization parameter λ_θ in the helicity frame for direct $J/\psi, \psi(2S)$, and Υ compared to CMS measurements [45,46].

large p_T. We consider the polarization parameter λ_θ in the helicity frame, which takes values $+1$, 0, and -1 when the quarkonium is transverse, unpolarized, and longitudinal, respectively [42–44]. The pNRQCD expressions for the CO LDMEs in Eqs. (4) imply that the polarization of directly produced quarkonium is independent of the radial excitation, up to corrections of higher orders in v^2. Although the ${}^3S_1^{[8]}$ and ${}^3P_J^{[8]}$ channels are strongly transverse, the large cancellation between the two channels result in smaller values of λ_θ. Because $\mathcal{E}_{00}$ is positive, we expect that Υ is more transverse than J/ψ or $\psi(2S)$ at comparable values of p_T/m, due to the running of $\mathcal{E}_{10;10}$ which makes it take a greater value at the scale of the bottom quark mass compared to the charmonium case. These expectations are supported by the pNRQCD results for λ_θ in the helicity frame shown in Fig. 2, which also agree with CMS measurements [45,46].

Other observables that provide tests of the CO LDMEs include production rates of J/ψ at ep and lepton colliders, and production of η_c. As have been pointed out in Refs. [47,48], many LDME determinations based on hadroproduction data are known to overestimate these cross sections compared to the measurements in Refs. [49–52]. A small or negative value of $\langle \mathcal{O}^{J/\psi}({}^1S_0^{[8]})\rangle$, similar to what we obtain from our result for $c_F^2 \mathcal{B}_{00}$, can reduce the size of these cross sections compared to existing hadroproduction-based approaches in Refs. [14,16,20,53], diminishing in this way the tension with measurements [54].

The pNRQCD calculation of the NRQCD LDMEs of S-wave heavy quarkonia that we have presented in this paper provides expressions for the color-singlet and color-octet LDMEs in terms of quarkonium wave functions and universal gluonic correlators. This brings in a reduction of the number of nonperturbative unknowns and significantly enhances the predictive power of the factorization formalism for inclusive production of heavy quarkonia. The universality of the gluonic correlators lets us determine the LDMEs from charmonium and bottomonium data, which leads to strong constraints on the LDMEs. Especially, the P-wave CO LDMEs are strongly constrained, which may be more robust against radiative corrections compared to existing determinations. The pNRQCD results for the inclusive cross sections of J/ψ, $\psi(2S)$, and excited Υ states and their polarizations at the LHC are shown in Figs. 1 and 2. They agree with measurements at the LHC. More measurements of production rates of excited Υ states at large p_T will help further reduce theoretical uncertainties. The pNRQCD calculation of the NRQCD LDMEs for production of S-wave heavy quarkonia presented in this paper may be important in resolving the longstanding puzzle of the heavy quarkonium production mechanism.

We thank Peter Vander Griend for his careful reading of the manuscript. The work of N. B. is supported by the DFG (Deutsche Forschungsgemeinschaft, German Research Foundation) Grant No. BR 4058/2-2. N. B., H. S. C., and A. V. acknowledge support from the DFG cluster of excellence "ORIGINS" under Germany's Excellence Strategy—EXC-2094–390783311. The work of A. V. and X.-P. W. is funded by the DFG Project-ID 196253076—TRR 110.

[1] N. Brambilla *et al.* (Quarkonium Working Group), Report Nos. CERN-2005-005, CERN-2005-005, CERN, Geneva, 2005.
[2] N. Brambilla *et al.*, Eur. Phys. J. C **71**, 1534 (2011).
[3] G. T. Bodwin, E. Braaten, E. Eichten, S. L. Olsen, T. K. Pedlar, and J. Russ, in *Community Summer Study 2013: Snowmass on the Mississippi* (2013), arXiv:1307.7425.
[4] N. Brambilla *et al.*, Eur. Phys. J. C **74**, 2981 (2014).

[5] W. E. Caswell and G. P. Lepage, Phys. Lett. **167B**, 437 (1986).
[6] G. T. Bodwin, E. Braaten, and G. P. Lepage, Phys. Rev. D **51**, 1125 (1995); **55**, 5853(E) (1997).
[7] G. C. Nayak, J.-W. Qiu, and G. F. Sterman, Phys. Lett. B **613**, 45 (2005).
[8] G. C. Nayak, J.-W. Qiu, and G. F. Sterman, Phys. Rev. D **72**, 114012 (2005).
[9] G. C. Nayak, J.-W. Qiu, and G. F. Sterman, Phys. Rev. D **74**, 074007 (2006).
[10] Z.-B. Kang, Y.-Q. Ma, J.-W. Qiu, and G. Sterman, Phys. Rev. D **90**, 034006 (2014).
[11] Y.-Q. Ma, K. Wang, and K.-T. Chao, Phys. Rev. D **84**, 114001 (2011).
[12] M. Butenschoen and B. A. Kniehl, Phys. Rev. Lett. **106**, 022003 (2011).
[13] Y.-Q. Ma, K. Wang, and K.-T. Chao, Phys. Rev. Lett. **106**, 042002 (2011).
[14] K.-T. Chao, Y.-Q. Ma, H.-S. Shao, K. Wang, and Y.-J. Zhang, Phys. Rev. Lett. **108**, 242004 (2012).
[15] M. Butenschoen and B. A. Kniehl, Phys. Rev. Lett. **108**, 172002 (2012).
[16] B. Gong, L.-P. Wan, J.-X. Wang, and H.-F. Zhang, Phys. Rev. Lett. **110**, 042002 (2013).
[17] M. Butenschoen and B. A. Kniehl, Phys. Rev. D **84**, 051501 (2011).
[18] M. Butenschoen and B. A. Kniehl, Phys. Rev. Lett. **104**, 072001 (2010).
[19] M. Butenschoen and B. A. Kniehl, Phys. Rev. Lett. **107**, 232001 (2011).
[20] G. T. Bodwin, H. S. Chung, U.-R. Kim, and J. Lee, Phys. Rev. Lett. **113**, 022001 (2014).
[21] G. T. Bodwin, K.-T. Chao, H. S. Chung, U.-R. Kim, J. Lee, and Y.-Q. Ma, Phys. Rev. D **93**, 034041 (2016).
[22] H. S. Chung, Proc. Sci., Confinement2018 (2018) 007.
[23] N. Brambilla, H. S. Chung, and A. Vairo, Phys. Rev. Lett. **126**, 082003 (2021).
[24] N. Brambilla, H. S. Chung, and A. Vairo, J. High Energy Phys. 09 (2021) 032.
[25] A. Pineda and J. Soto, Nucl. Phys. B, Proc. Suppl. **64**, 428 (1998).
[26] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Nucl. Phys. **B566**, 275 (2000).
[27] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Rev. Mod. Phys. **77**, 1423 (2005).
[28] E. Eichten and B. R. Hill, Phys. Lett. B **243**, 427 (1990).
[29] A. Czarnecki and A. G. Grozin, Phys. Lett. B **405**, 142 (1997); **650**, 447(E) (2007).
[30] A. G. Grozin, P. Marquard, J. H. Piclum, and M. Steinhauser, Nucl. Phys. **B789**, 277 (2008).
[31] G. T. Bodwin, U.-R. Kim, and J. Lee, J. High Energy Phys. 11 (2012) 020.
[32] N. Brambilla, D. Eiras, A. Pineda, J. Soto, and A. Vairo, Phys. Rev. D **67**, 034018 (2003).
[33] S. Chatrchyan *et al.* (CMS Collaboration), J. High Energy Phys. 02 (2012) 011.
[34] V. Khachatryan *et al.* (CMS Collaboration), Phys. Rev. Lett. **114**, 191802 (2015).
[35] G. Aad *et al.* (ATLAS Collaboration), Phys. Rev. D **87**, 052004 (2013).
[36] M. Ablikim *et al.* (BESIII Collaboration), Phys. Rev. D **85**, 112008 (2012).
[37] N. Brambilla, H. S. Chung, D. Müller, and A. Vairo, J. High Energy Phys. 04 (2020) 095.
[38] L.-P. Wan and J.-X. Wang, Comput. Phys. Commun. **185**, 2939 (2014).
[39] G. Aad *et al.* (ATLAS Collaboration), J. High Energy Phys. 07 (2014) 154.
[40] R. Aaij *et al.* (LHCb Collaboration), Eur. Phys. J. C **74**, 3092 (2014).
[41] M. Tanabashi *et al.* (Particle Data Group), Phys. Rev. D **98**, 030001 (2018).
[42] M. Beneke and M. Krämer, Phys. Rev. D **55**, R5269 (1997).
[43] M. Beneke, M. Krämer, and M. Vanttinen, Phys. Rev. D **57**, 4258 (1998).
[44] P. Faccioli, C. Lourenço, J. a. Seixas, and H. K. Wöhri, Eur. Phys. J. C **69**, 657 (2010).
[45] S. Chatrchyan *et al.* (CMS Collaboration), Phys. Rev. Lett. **110**, 081802 (2013).
[46] S. Chatrchyan *et al.* (CMS Collaboration), Phys. Lett. B **727**, 381 (2013).
[47] M. Butenschoen and B. A. Kniehl, Mod. Phys. Lett. A **28**, 1350027 (2013).
[48] M. Butenschoen, Z.-G. He, and B. A. Kniehl, Phys. Rev. Lett. **114**, 092004 (2015).
[49] R. Aaij *et al.* (LHCb Collaboration), Eur. Phys. J. C **75**, 311 (2015).
[50] C. Adloff *et al.* (H1 Collaboration), Eur. Phys. J. C **25**, 25 (2002).
[51] P. Pakhlov *et al.* (Belle Collaboration), Phys. Rev. D **79**, 071101 (2009).
[52] F. D. Aaron *et al.* (H1 Collaboration), Eur. Phys. J. C **68**, 401 (2010).
[53] G. T. Bodwin, H. S. Chung, U.-R. Kim, and J. Lee, Phys. Rev. D **92**, 074042 (2015).
[54] N. Brambilla, H. S. Chung, X.-P. Wang, and A. Vairo, TUM-EFT 170/22 (to be published).