We calculate the cross section for hadroproduction of a pair of heavy quarks in a $^3S_1$ color-singlet state at next-to-leading order in QCD. This corresponds to the leading contribution in the NRQCD expansion for $J/\psi$ and $\Upsilon$ production. The higher-order corrections have a large impact on the $p_T$ distributions, enhancing the production at high $p_T$ both at the Tevatron and at the LHC. The total decay rate of a $^3S_1$ into hadrons at NLO is also computed, confirming for the first time the result obtained by Mackenzie and Lepage in 1981.

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1. Charmonium and bottomonium states are certainly among the most interesting systems to test our understanding of the strong interactions, both at the perturbative and non-perturbative level. More than thirty years after the discovery of the first charm-anticharm resonance, the $J/\psi$, the study of their properties, including production and decay mechanisms, is still the subject of considerable interest [1].

From the theoretical point of view, a rigorous framework, based on the use of non-relativistic QCD (NRQCD) [2], has been introduced that allows consistent theoretical predictions to be made and to be systematically improved. However, despite theoretical developments and successes, not all the predictions of the NRQCD factorization approach have been firmly established. Recent measurements in $e^+e^-$ collisions have shown that production rates for single and double charmonium production are in general much larger than those predicted by leading order calculations [3]. Measurements at the Tevatron in proton-antiproton collisions are not fully compatible with those obtained at HERA in electron-proton collisions [4] and in fixed-target experiments [5], suggesting the possibility that charmonium might be too light for the NRQCD factorization and/or scaling rules to work. In this context, a real challenge is offered by measurements of the $J/\psi$ polarization at the Tevatron. NRQCD predicts a sizeable transverse polarization for $J/\psi$'s at high-$p_T$, in contrast with the latest data that now clearly indicate that $J/\psi$'s are not transversely polarized [6].

In view of such a puzzling scenario, it is worth to re-examine in detail the theoretical predictions and try to systematically improve on them. In this Letter we report on the calculation of the next-to-leading order correction to the hadroproduction of a pair of heavy quarks in a color-singlet $^3S_1$ state. This is the leading term in the NRQCD expansion for a $J/\psi$ or a $\Upsilon$ and it is equivalent to the "color-singlet model" approximation. This model assumes that the non-perturbative dynamics leaves unchanged the quantum numbers of the perturbative quark-antiquark pair, which are the same as those of the physical bound state. It is curious to note that the analogous corrections to the hadronic decay width of a color-singlet $^3S_1$ state, which involve exactly the same diagrams, have been available for a long time [7] and play an important role in the extraction of $\alpha_S$ from $\Upsilon$ decays [8]. Our calculation for the inclusive decay rate at NLO provides the first independent confirmation of those results.

2. According to the NRQCD factorization approach [2], the inclusive cross section for direct production for a $J/\psi$, $\Upsilon$ and their radial excitations, (hereafter denoted $Q$) in hadron-hadron collisions can be written as:

$$\sigma(pp \to Q + X) = \sum_{i,j,n} \int dx_1 dx_2 f_i/p f_j/p \int dx \hat{\sigma}[ij \to (Q\bar{Q})_n + x]|0| \langle 0| O_n^{ij} |0 \rangle,$$

FIG. 1: Representative Feynman diagrams for $^3S_1$ hadroproduction at LO (a), virtual (b), and real (c) contributions at NLO. Amplitudes with a light quark line (not shown) also contribute to the real corrections.
where \( p \) is either a proton or an antiproton. The short-distance coefficients \( \hat{\sigma} \) are calculable in perturbative QCD and describe the production of a heavy quark–antiquark pair \( QQ \) state with quantum numbers \( n \). Conversely, the \( \langle 0|O_n^S|0 \rangle \) are the non-perturbative matrix elements that describe the subsequent hadronization of the \( QQ \) pair into the physical \( Q \) state. These matrix elements can be expanded in powers of the relative velocity of the heavy quarks in the bound state, \( v^2 \). Since \( v^2 \approx 0.3(0.1) \) for charmonium (bottomonium) only a few terms need to be included in the sum over \( n \) to reach a given accuracy. Compared to the leading contribution, the \( ^3S_1^{[1]}(QQ) \), the color-octet terms, \( \langle 1S_0^{[8]}|3S_1^{[8]}|3p_0^{[8]} \rangle \), are all suppressed by \( v^4 \). However, the corresponding short distance coefficients might compensate this suppression, either by having leading order contributions starting at \( \alpha_s^2 \) compared to the \( \alpha_s^3 \) of the singlet and/or by kinematic enhancements due to a different scaling of the differential cross section with the \( p_T \). In particular it is easy to verify that the partonic differential cross sections at LO behave as \( 1/p_T^5 \) for CP-even color-octet states and \( 1/p_T^4 \) for the \( ^3S_1^{[8]} \), compared to the \( 1/p_T^8 \) scaling of the color-singlet. In the case of charmonium production at the Tevatron, the \( 1/p_T^4 \) and \( 1/p_T^5 \) behaviors are clearly seen in the data [4] and the introduction of the contribution from the octets allows explanation of the observed \( p_T \) spectrum [11]. On the other hand, at NLO \( ^3S_1^{[1]} \) production has both \( 1/p_T^6 \) and \( 1/p_T^5 \) components, the latter coming from the associated production with a heavy-quark pair, that can affect the interpretation of these behaviors in terms of color-octet matrix elements [11].

3. Analogously to orthopositronium in QED, for a \( ^3S_1 \) state the first non-zero contribution in QCD comes from the coupling to three gauge vectors, so that in hadron collisions the quarkonium is produced in association with a gluon, Fig. II(a). Since we want to retain spin-correlations and work with helicity amplitudes, we find it convenient to include the decay of the quarkonium state in to a pair of leptons, \( \ell \ell \). In so doing the projection of the quantum numbers (color and spin) of the heavy-quark pair to a \( ^3S_1^{[1]} \) state is automatic. The color-ordered helicity amplitudes for the short distance process \( ggg \to ^3S_1^{[1]} \to \ell \ell \) are

\[
A(1^+,2^+,3^+,5^+_t,6^-_t) = 0, \\
A(1^+,2^+,3^-,5^+_t,6^-_t) = \frac{\mathcal{N}}{(s_{12} + s_{13})(s_{13} + s_{23})(s_{12} + s_{23})} (35)^2[12]^2[56],
\]

where \( \mathcal{N} = 8\sqrt{2}g_s^3a^2m_Q \).

Next-to-leading order corrections include virtual corrections to the \( 2 \to 2 \) process, Fig. II(b), the real processes, such as the purely gluonic contribution \( gg \to Qgq \), Fig. II(c). In addition, channels with a quark-antiquark pair: \( gg \to Qqg \) and their crossings also contribute.

The amplitudes \( gggg, gggq \to ^3S_1^{[1]} \to \ell \ell \) which enter the real corrections, have been calculated analytically and checked numerically against those obtained with MadGraph [12]. We note that by squaring the full amplitudes involving four gluons and summing over color we find a non-trivial simplification, with only one kinematical combination. The overall color coefficient is given by \( N_cC_2(F) \), with \( C_2(F) \) being the second Casimir of \( SU(3) \) and corresponding to the color factor of the Born squared amplitude, i.e., \( C_2(F) = (d^{abc}/\sqrt{N_c})^2 \).

Virtual corrections to the leading order helicity amplitudes have been calculated within the four dimensional helicity scheme. Dimensional regularization has been adopted for isolating the ultraviolet, infrared and collinear singularities. The heavy-quark mass and wave function have been renormalized on-shell. \( M \hat{S} \) renormalization has been employed for the gluon wave function and \( \alpha_S \) renormalization. The color projection onto a singlet state leads to remarkable simplifications at NLO. We split diagrams containing the four-gluon vertex into a sum of color ordered terms, where each term is written as a product of color matrices in the fundamental representation, \( \lambda^a \). In this way each virtual diagram contributes to all of the six gluon permutations each multiplying \( \text{Tr}(\lambda^a \lambda^b \lambda^c) \). In fact, out of the above six permutations, only one independent combination is left which is the sum of three permutations with the same order of the color generators. The full amplitudes are proportional to \( d^{abc}/\sqrt{N_c} \), exactly as for the Born amplitude. Thus all the contributions from individual diagrams for each helicity configuration can be summed together, resulting in a sizeable simplification of analytic expressions for the final results. We also find that the infrared divergences are proportional to \( N_c \), while the subleading terms in \( N_c \) are finite, in agreement with the simplifications mentioned above for the real corrections. As a further check of our calculation, we verified numerically the identity of the two color ordered subamplitudes and their gauge invariance under different choices for the polarization vectors of the three gluons.

To extract the singularities of the real part of the NLO corrections \( \sigma^{\text{real}} \), the dipole subtraction formalism [15] has been adopted, following the implementation of MCFM [14]. The algorithm is based
FIG. 2: Variation of the cross section for direct $\Upsilon$ production at the Tevatron (lower curves) and the LHC (upper curves) at LO (dashes) and NLO (solid). Renormalization and factorization scales are set equal, $\mu_F = \mu_R$, and $\mu_0 = \sqrt{(2m_b)^2 + p_T^2}$.

on mapping the singularities of the real cross section $\sigma_{\text{real}}$ onto an auxiliary cross section $\sigma_{\text{aux}}$ which can be built out of universal building blocks, the so-called dipoles, and it is simple enough that the singular regions in phase space can be integrated out analytically. The remaining piece, $\sigma_{\text{real}} - \sigma_{\text{aux}}$ is finite and can be safely integrated with standard Monte Carlo techniques. The divergences in the auxiliary cross section $\sigma_{\text{aux}}$ are in part canceled by the the soft and collinear singularities of the virtual corrections while the rest are absorbed in the renormalization of the parton densities. Note that no dipoles for the heavy quarks are needed since there are no infrared divergences associated with a collinear heavy quark-antiquark pair in a color-singlet state. Indeed we find that the structure of the infrared divergences is the same as that of Higgs hadroproduction in association with a jet [15], as it should be.

4. We now turn to the presentation of the main features of the NLO results. In our numerical studies, the CTEQ6L1 (CTEQ6M) parton distribution functions and the corresponding fitted value for $\alpha_S(M_Z) = 0.130(0.118)$ are used for the LO (NLO) predictions. The heavy-quark mass and the color-singlet non-perturbative matrix element are $\langle O_T^{(3S_1)} \rangle = 9.28 \text{ GeV}^3$ and $m_c = 4.75 \text{ GeV}$ for the $\Upsilon$, and $\langle O_T^{(J/\psi)}(3S_1) \rangle = 1.16 \text{ GeV}^3$ and $m_c = 1.5 \text{ GeV}$ for the $J/\psi$.

The inclusion of the NLO corrections leads to important modifications of the total cross sections and the distributions. First we note that, even though the calculation of the total cross section at NLO is infrared-safe, there are some regions of the phase space, notably at low $p_T$ and at large rapidity of the quarkonium state, where the perturbative expansion is not under proper control and a fixed-order approximation fails to provide a reliable estimate. This is the same behavior found in the corresponding regions of the phase space in the calculation for $\gamma p \to 3S_1^{[1]} + X$ at NLO [16]. A careful treatment of the effects of soft radiation as outlined, e.g., in Ref. [17] is beyond the scope of this Letter and is left for future work. For the sake of illustration, we restrict our results to the domain $p_T^2 > 3 \text{ GeV}^2$ and $|y^Q| < 3$ where the cross section is always positive definite. We then study how the calculation behaves by looking at the dependence of the cross section on the input parameters.

FIG. 3: Variation of the cross section for direct $J/\psi$ production at the Tevatron (lower curves) and the LHC (upper curves) at LO (dashes) and NLO (solid). Renormalization and factorization scales are set equal $\mu_F = \mu_R$, and $\mu_0 = \sqrt{(2m_c)^2 + p_T^2}$.

FIG. 4: Differential cross sections for direct $\Upsilon$ production via a $3S_1^{[1]}$ intermediate state, at the Tevatron (lower histograms) and LHC (upper histograms), at LO (dashes) and NLO (solid). $p_T^2 > 3 \text{ GeV}^2$ and $|y^Q| < 3$. Details on the input parameters are given in the text.
FIG. 5: Differential cross sections for direct \( J/\psi \) production via a \( ^3S_1 \) intermediate state, at the Tevatron (lower histograms) and LHC (upper histograms), at LO (dashes) and NLO (solid). \( p_T^{J/\psi} > 3 \text{ GeV} \) and \( |y^{J/\psi}| < 3 \).

Details on the input parameters are given in the text.

section on variations of the renormalization and factorization scales between \( \mu_0/2 < \mu_F = \mu_R < 2\mu_0 \), with \( \mu_0 = \sqrt{(2m_Q)^2 + p_T^2} \). The results are shown in Figs. 2 and 3. We find that the NLO prediction for \( \Upsilon \) production is very well behaved both at Tevatron and the LHC and the scale dependence is (slightly) improved. For \( J/\psi \) the scale dependence at NLO is not improved in this region of the phase space.

In Figs. 4 and 5 we plot the inclusive \( p_T \) distributions of the quarkonium states, with \( p_T^{Q} > 3 \text{ GeV} \) and \( |y^{Q}| < 3 \). Details on the input parameters are given in the text.

\[ \Gamma^{\text{NLO}}(\Upsilon \to LH) = \Gamma^{\text{LO}} \left[ 1 + \frac{\alpha_S(\mu)}{\pi} \left( -9.471 C_F + 4.106 C_A - 1.150 n_f + \frac{3}{2} \beta_0 \log \frac{\mu}{m_b} \right) \right], \]

with \( \beta_0 = \frac{11}{3} C_A - \frac{2}{3} n_f \) and \( C_F = 4/3, C_A = 3 \). The numerical coefficients, obtained by a Monte Carlo integration method, have an uncertainty better than one per mil, and are in good agreement with those of Ref. [7]. Eq. (3) provides the first independent check of the results of that seminal work.

5. To summarize, we have presented the NLO cross section for the production of a heavy quark pair in a \( ^3S_1 \) state at hadron colliders. This is the leading contribution in the relative velocity expansion to the production of \( J/\psi, \Upsilon \) and their radial excitations. The NLO corrections are large and modify the expectations for the total cross sections and the distribution in the transverse momentum. Further analysis, including combination with the results of Ref. [18] for \( pp \to QQ \) and Ref. [19], to compare with the available data from the Tevatron and fixed-target experiments is the subject of a forthcoming paper.

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