Scale-Fixed Predictions for $\gamma + \eta_c$ production in electron-positron collisions at NNLO in perturbative QCD

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In the paper, we present QCD predictions for $\eta_c + \gamma$ production at an electron-positron collider up to next-to-next-to-leading order (NNLO) accuracy without renormalization scale ambiguities. The NNLO total cross-section for $e^+e^- \rightarrow \gamma + \eta_c$, using the conventional scale-setting approach has large renormalization scale ambiguities, usually estimated by choosing the renormalization scale to be the $e^+e^-$ center-of-mass collision energy $\sqrt{s}$. The Principle of Maximum Conformality (PMC) provides a systematic way to eliminate such renormalization scale ambiguities by summing the nonconformal $\beta$ contributions into the QCD coupling $\alpha_s(Q^2)$. The renormalization group equation then sets the value of $\alpha_s$ for the process. The PMC renormalization scale reflects the virtuality of the underlying process, and the resulting predictions satisfy all of the requirements of renormalization group invariance, including renormalization scheme invariance. After applying the PMC, we obtain a scale-and-scheme independent prediction, $\sigma_{\text{NNLO,PMC}} \simeq 41.18$ fb for $\sqrt{s}=10.6$ GeV. The resulting pQCD series matches the series for conformal theory and thus has no divergent renormalon contributions. The large $K$ factor which contributes to this process reinforces the importance of uncalculated NNLO and higher-order terms. Using the PMC scale-and-scheme independent conformal series and the Padé approximation approach, we predict $\sigma_{\text{NNLO,PMC+Padé}} \simeq 21.36$ fb, which is consistent with the recent BELLE measurement $\sigma_{\text{exp}}^{\eta_c} = 16.58^{+10.53}_{-9.93}$ fb at $\sqrt{s} \simeq 10.6$ GeV. This procedure also provides a first estimate of the NNNLO contribution.

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I. INTRODUCTION

Processes involving the production of heavy quarkonium are important for testing Quantum Chromodynamics (QCD) as well as the effective theory of Nonrelativistic QCD (NRQCD) \cite{1}. The framework of NRQCD factorization theory allows the non-perturbative dynamics involving the binding of the heavy quark-antiquark pair in quarkonium to be factored into universal NRQCD matrix elements which can be extracted and fixed via a global fitting of experiments involving heavy quarkonium production. The remaining ‘hard’ contribution involving high momentum transfers is then perturbatively calculable. Thus reliable calculations of quarkonium production and its decay now appear viable.

The NRQCD approach has been successfully applied to a number of quarkonium processes, but many challenges and puzzles have remained. At present, most NRQCD results have been done at the next-to-leading order (NLO) level. Next-to-next-to-leading order (NNLO) and higher-order calculations are much more difficult. Thus it is important to test a variety of NNLO predictions before drawing any definite conclusion on the general applicability of NRQCD, especially since the $K$ factors which appear in quarkonium production processes can be very large.

The production of the $\eta_c$ via $e^+ + e^- \rightarrow \gamma + \eta_c$ is an important charmonium production process which can be precisely measured at high-energy, high-luminosity electron-positron colliders. For example, the Belle II experiment is expected to produce a sizable number of $\gamma + \eta_c$ events in the near future, which can be used to make precise comparisons with theoretical predictions. This heavy quarkonium production process has been calculated in pQCD up to NNLO level \cite{3,4,5,6}. However, the NNLO calculation performed by Chen, Liang and Qiao \cite{7} displays both a large $K$ factor and large renormalization scale uncertainties. As a cross check, and also as important step forward, we shall recalculate the $e^+ + e^- \rightarrow \gamma + \eta_c$ cross section at NNLO level, make a detailed discussion on how to eliminate the unnecessary renormalization scale ambiguities, and present a first prediction of the NNNLO contribution.

A physical observable, corresponding to an infinite-order pQCD approximate, is independent of the choice of renormalization scale. If the perturbative coefficients and the strong coupling constant $\alpha_s$ are not well matched at a fixed order, as is the case of conventional scale-setting approach in which the renormalization scale is simply guessed, one finds significant renormalization scale-and-scheme ambiguities; cf. the reviews \cite{8,9,10}. Any dependence of pQCD prediction on the choice of renormalization scheme violates a fundamental principle of the renormalization group. In fact, predictions based on conventional scale setting are even incorrect for Abelian theory – Quantum Electrodynamics (QED); the renormalization scale of the QED coupling constant $\alpha$ can be set unamb-

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biguously by using the Gell-Mann-Low method [11]. It is thus essential to use a rigorous scale-setting approach in order to achieve reliable and precise scale-and-scheme independent fixed-order pQCD predictions.

The Principle of Maximum Conformality (PMC) [12–16] provides a rigorous approach to renormalization scale setting, extending the BLM method [17] to all orders in pQCD. The purpose of the PMC is not to find an ‘optimal’ renormalization scale, but to systematically and rigorously determine the renormalization scale and thus the effective value of \( \alpha_s \) consistent with the renormalization group equation (RGE). After applying the RGE, the resulting pQCD prediction is independent of the choice of the renormalization scheme. The scheme-dependent non-conformal \( \{ \beta_i \} \)-terms are eliminated in the pQCD series, which matches the corresponding conformal series. The commensurate scale relations [18] which relate PMC predictions for different observables to each other are also scheme independent. The PMC procedure reduces in the \( N_C \to 0 \) Abelian limit to the Gell-Mann-Low method [19]. Thus the PMC eliminates renormalization scale-and-scheme ambiguities simultaneously, satisfying the principles of renormalization group invariance [20, 21]. In addition, since the \( \{ \beta_i \} \)-terms have been removed, the divergent renormalon terms like \( \alpha_s^2 \beta_0 n! \) disappear and a convergent perturbative series can be naturally achieved.

In the paper, we shall adopt the PMC single-scale approach [22] for our analysis. The PMC scale can be interpreted as the effective momentum flow within the production process; its value displays stability and convergence with increasing order in pQCD, and any residual scale dependence due to unknown higher-order terms is highly suppressed.

The remaining parts of the paper are organized as follows: In Section II, we give the calculation technology for the total cross section of \( e^+ e^- \to \gamma + \eta_c \) at NNLO level. We present the numerical results in Section III, and Section IV is reserved for the summary.

\[ \begin{align*}
K &|_{m_c=1.4 GeV} = 1 - 2.40418a_s(\mu_r) + [-80.106 - 37.28517 \log \frac{\mu_A^2}{m_c^2} + (-6.21079 + 0.40070 \times n_l) \log \frac{\mu_r^2}{m_c^2} \\
&+ 1.87 \times \mu_r + 2.02242 \times n_l - 1.90725 \times lbb + n_l a_s(\mu_r),
\end{align*} \]

\[ \begin{align*}
K &|_{m_c=1.5 GeV} = 1 - 2.56853a_s(\mu_r) + [-80.09 - 37.28517 \log \frac{\mu_A^2}{m_c^2} + (-6.63538 + 0.42809 \times n_l) \log \frac{\mu_r^2}{m_c^2} \\
&+ 2.12 \times \mu_r - 1.95854 \times n_l - 1.79911 \times lbb + n_l a_s(\mu_r),
\end{align*} \]

\[ \begin{align*}
K &|_{m_c=1.6 GeV} = 1 - 2.72207a_s(\mu_r) + [-80.193 - 37.28517 \log \frac{\mu_A^2}{m_c^2} + (-7.03202 + 0.45368 \times n_l) \log \frac{\mu_r^2}{m_c^2} \\
&+ 2.354 \times \mu_r - 1.89264 \times n_l - 1.69825 \times lbb + n_l a_s(\mu_r),
\end{align*} \]

where \( \mu_A \) is the factorization scale, \( n_l \) is the number of light flavors (u, d and s), and “lbb” denotes the contri-
bution from the light-by-light Feynman diagrams. The \( bbl \)-terms are free of ultra-violet (UV) and are irrelevant to the running of \( \alpha_s \), so they should be kept as conformal terms when applying the PMC. Using the above equations, the coefficients \( r_i \) can be fixed.

In order to apply the PMC, the coefficients \( r_i \) need to be divided into conformal terms and non-conformal terms [15, 16], and for the present NNLO analysis, the coefficients for the perturbative series (1) can be written as

\[
\begin{align*}
    r_1 &= r_{1,0}, \\
    r_2 &= r_{2,0} + r_{2,1} \beta_0,
\end{align*}
\]

where \( \beta_0 = 11 - 2/3n_f \) with the active flavor numbers \( n_f = n_l + 1 \) (\( n_f = 4 \) for \( \eta_c \) production). The coefficients \( r_{1,0} \) are the conformal coefficients and the \( r_{1,j \neq 0} \) are non-conformal ones. By using the standard PMC scale-setting procedures, the NNLO total cross section (1) can be written as a conformal series,

\[
\sigma = \sigma^{(0)}[1 + r_{1,0} \alpha_s(Q_s) + r_{2,0} \alpha_s^2(Q_s)],
\]

where \( Q_s \) stands for the PMC scale which is determined by requiring all non-conformal terms to vanish. The PMC scale can be fixed up to leading-log (LL) accuracy by using the known NNLO pQCD series; i.e.,

\[
\ln \frac{Q^2}{m_c^2} = - \frac{\hat{r}_{2,1}}{r_{1,0}} + O(\alpha_s),
\]

where \( \hat{r}_{2,1} = r_{2,1} |_{\mu_r = m_c} \).

The PMC scale \( Q_s \) can be regarded as the effective momentum flow of the process, since it is determined by using the RGE and the effective value of \( \alpha_s(Q_s) \) has been fixed. Eq. (11) shows that the scale \( Q_s \) is independent of the choice of \( \mu_r \). Since the conformal coefficients \( r_{1,0} \) are scale-independent, the PMC prediction is exactly free of \( \mu_r \)-dependence. Thus the conventional renormalization scale ambiguity is solved.

The unknown higher-order terms in the perturbative series of \( \ln Q^2/m_c^2 \) can have some residual scale dependence [24]; however, this dependence is distinct from the conventional renormalization scale ambiguities, and it has both \( \alpha_s \)-power suppression and exponential suppression. In practice, most applications of the PMC published in the literature show that such residual scale dependence is rather small [8, 10].

### III. NUMERICAL RESULTS

For doing the numerical analysis, we will take \( \alpha = 1/130.7, \alpha_s(M_Z) = 0.1181 \) [26], \( \sqrt{s} = 10.6 \text{ GeV} \), and the \( \eta_c \) matrix element \( \langle O_1 | S_0 \rangle |_{\mu_A = 1 \text{ GeV}} = 0.437 \text{ GeV}^3 \) [27, 28]. The required two-loop \( \alpha_s \) running is calculated by using the RunDec program [29].

| \( K \) factor | LO | NLO | NNLO | Total |
|--------------|-----|-----|------|-------|
| Conv. 1     | -0.14±0.02 | -0.28±0.05 | 0.61±0.07 | -0.10 |
| PMC 1       | -0.13 | -0.23 | 0.64  |       |

TABLE I: The \( K \) factors using the conventional and PMC scale-setting approaches up to NNLO level. The labels “LO”, “NLO” and “NNLO” stand for the contributions of the LO, the NLO and the NNLO terms, respectively. \( \mu_A = 1 \text{ GeV} \). The central values are for \( \mu_r = \sqrt{s} \) and the errors are for \( \mu_r \in [\sqrt{s}/2, 2\sqrt{s}] \) for conventional scale-setting. The PMC predictions are independent of the choice of \( \mu_r \).

Assuming \( m_c = 1.5 \text{ GeV} \) and the factorization scale \( \mu_A = 1 \text{ GeV} \), the total cross sections under conventional scale-setting approach (Conv.) for three typical choices of renormalization scale are

\[
\begin{align*}
    \sigma^{\text{Conv}}_{\text{NNLO}} |_{\mu_r = \sqrt{s}/2} &= 0.51 \sigma^{(0)}, \\
    \sigma^{\text{Conv}}_{\text{NNLO}} |_{\mu_r = \sqrt{s}} &= 0.61 \sigma^{(0)}, \\
    \sigma^{\text{Conv}}_{\text{NNLO}} |_{\mu_r = 2\sqrt{s}} &= 0.68 \sigma^{(0)},
\end{align*}
\]

which shows that the conventional scale uncertainty is about \( +11.5\% \) \(-16.3\% \) for \( \mu_r \in [\sqrt{s}/2, 2\sqrt{s}] \). On the other hand, since the PMC scale \( Q_s \) is fixed to be 14.78 GeV, the total cross section using PMC scale-setting approach is independent of the choice of \( \mu_r \); i.e.

\[
\sigma^{\text{PMC}}_{\text{NNLO}} \equiv 0.64 \sigma^{(0)}.
\]

Table I shows how the magnitude of each loop term changes with different choices of \( \mu_r \). After applying the PMC, the scale dependence of each loop term is eliminated; however, the pQCD convergence is still poor. This

\[1 \text{ In some cases where both the resulting conformal series and the perturbative series of the PMC scale do not converge well, the residual scale dependence may be large. This dependence is expected to be suppressed when one includes higher loop terms. An example can be found for Higgs-boson decay } H \rightarrow gg \text{ [25].}]}
is due to the fact that the conformal coefficient is large and dominates over the total NNLO coefficient $r_2$, e.g. $r_2 = -79.9 \pm 7.4$ where $r_{2,0} \equiv -83.5$ for $\mu_r \in [\sqrt{s}/2, 2\sqrt{s}]$.

We have observed numerically that if one sets $\mu_r = \sqrt{2s}$, the conventional prediction gives total cross section and perturbative behavior which are close in comparison to the PMC prediction; thus $\sqrt{2s}$ can be treated as the optimal renormalization scale of conventional prediction.

Fig. (1) shows how the net scale uncertainty varies when more loop terms have been included. Contrary to usual expectations, the net NNLO scale uncertainty of the conventional series is larger than that of the NLO series, since cancellations of terms at different orders are absent. In contrast, after applying the PMC, both the NLO and NNLO $K$ factors are free of the renormalization scale ambiguities. In this sense, the scale-invariant PMC conformal series is extremely important for precise pQCD predictions.

After eliminating the renormalization scale uncertainty, there are other error sources such as the factorization scale, the charm quark mass $m_c$, the value of $\alpha_s(M_Z)$, and the $\eta_c$ matrix element $\langle \mathcal{O}_1 | S_0 \rangle$. The matrix element is an overall parameter, whose error can be determined separately. Thus, in the following, we shall only discuss uncertainties which come from $\mu_A, m_c$ and $\Delta \alpha_s(M_Z)$. When discussing the uncertainty of the PMC prediction from one parameter, the other parameters are set as their central values.

First, to discuss the factorization scale uncertainty, we adopt $\mu_A=1$ GeV, $m_c$ and $2m_c$ with $m_c = 1.5$ GeV, respectively. The $K$ factors are

$$K^{\text{PMC}} = 0.64, \ 0.56, \ 0.42,$$

(16)

accordingly. Fig. (2) shows that the factorization scale dependence under conventional and PMC scale-setting approaches, respectively. It shows that the $K$ factor decreases with increasing factorization scale.

Second, to discuss the $m_c$ uncertainty, we adopt $m_c = 1.4, 1.5, \text{ and } 1.6$ GeV, respectively. By setting $\mu_A = 1$ GeV, we obtain

$$K^{\text{PMC}} = 0.65, \ 0.64, \ 0.63,$$

(17)

accordingly. Fig. (3) shows that the $m_c$ dependence under conventional and PMC scale-setting approaches, respectively. The $K$ factor decreases with the increment of $m_c$.

Third, to discuss the $\Delta \alpha_s(M_Z)$ uncertainty, we adopt $\Delta \alpha_s(M_Z) = 0.0011$. $m_c = 1.5$ GeV and $\mu_A = 1$ GeV.

$$K^{\text{PMC}} = 0.65, \ 0.64, \ 0.63,$$

(18)

accordingly. Fig. (4) shows that the $\Delta \alpha_s(M_Z)$ dependence under conventional and PMC scale-setting approaches, respectively.
We are now ready to discuss the properties of the total cross section. The PMC NNLO total cross section is

\[ \sigma_{\text{NNLO}}^{\text{PMC}} = 41.18^{+8.17}_{-11.83} + 4.76_{-3.92}^{+0.72} \text{ fb}, \]  

(19)

where the first error is for \( \mu_A \in [1, 3] \) GeV, the second error is for \( m_c \in [1.4, 1.6] \) GeV, and the third error is for \( \Delta \alpha_s(M_Z) = \pm 0.0011 \). The central value is for \( \mu_A = 1.5 \) GeV, \( \alpha_s(M_Z) = 0.1181 \), and \( (\Omega_1^{1S_0})|_{\mu_A=1.5\text{GeV}} = 0.418 \text{ GeV}^3 \), which is obtained by evolving the matrix element \( (\Omega_1^{1S_0})|_{\mu_A=1.0\text{GeV}} = 0.437 \text{ GeV}^3 \) from 1 GeV to 1.5 GeV with the help of the one-loop evolution formulae given in Ref.[1].

Recently, the BELLE Collaboration published their measured total cross-section for the process \( e^+e^- \rightarrow \eta_c + \gamma \) at \( \sqrt{s} = 10.58 \) GeV: \( \sigma_{\text{obs}} = 16.58^{+10.51}_{-9.95} \text{ fb} \) [37]. This value is smaller than the theoretical prediction (19). The central theoretical value shows a 2.3\( \sigma \) deviation from the data, which increases to 3.1\( \sigma \) when taking the usual choice of \( \mu_A = 1 \) GeV. If one takes the uncertainty of the \( \eta_c \) matrix element into consideration, e.g. \( \Delta (\Omega_1^{1S_0})|_{\mu_A=1.5\text{GeV}} = (0.111)_{-0.105}^{+0.110} \text{ GeV}^3 \) [27, 28], we then have an additional uncertainty, \( (10.94)_{-10.34}^{+10.94} \text{ fb} \), to the total cross section. This gives a slight overlap of the theoretical prediction with the measurement.

As a final remark, as shown by Table I, the poor pQCD convergence is due to the intrinsic nature of the present process, which cannot be improved even after applying the PMC. Thus it is necessary to know the contributions from unknown terms before we draw any definite conclusions. The conventional error estimate obtained by varying the guessed scale over a certain range cannot give a reliable prediction of the unknown terms, since it only partly estimates the non-conformal contribution but not the conformal one.

If one has a renormalization-scale independent conformal series, one can often obtain a reliable prediction of unknown higher-order contributions [30] with the help of the Padé resummation [31–33]. The diagonal [1/1]-type Padé series is generally preferable for estimating the unknown contributions from a poor pQCD convergent series [34–36]; and for the present process, the poor convergence of PMC series is due to large conformal coefficients. Detailed procedures for obtaining a combined Padé +PMC prediction can be found in Ref.[36]. By using the diagonal [1/1]-type PAA approximant, the predicted coefficient of the N^3LO term is -2713.77, which results in an extra 38% suppression from the LO cross-section, leading to a NNNLO prediction in better agreement with the data; i.e.,

\[ \sigma_{\text{NNNLO}}^{\text{PMC}} = 21.36 \text{ fb}, \]  

(20)

where \( \mu_A = 1 \) GeV and the other parameters are set to their central values. This indicates the importance of a strict NNNLO calculation, even though it would be much more difficult than the present NNLO calculation.

### IV. SUMMARY

In this paper, we have presented a detailed study of the cross section for \( \gamma + \eta_c \) production in electron-position collisions up to NNLO level. If one used the conventional procedure, the renormalization scale uncertainty for the NNLO total cross-section is estimated as 28% by varying the scale within the the range of \( \sqrt{s}/2, 2\sqrt{s} \). However, after applying PMC scale setting, the conventional scale uncertainty is eliminated.

Our NNLO prediction is,

\[ \sigma_{\text{NNLO}}^{\text{PMC}} = 41.18^{+9.48}_{-12.48} \text{ fb}, \]  

(21)

where the errors are squared average of the errors caused by varying \( \mu_A \in [1, 3] \) GeV, \( m_c \in [1.4, 1.6] \) GeV, and \( \Delta \alpha_s(M_Z) = \pm 0.0011 \). Among the uncertainties from the other input parameters, the factorization scale error is the largest. The central value of the NNLO cross section deviates substantially from the measured data. The poor pQCD convergence of the series indicates the importance of uncalculated NNNLO terms for this process. An initial estimate of the NNNLO terms with the help of the PMC and Padé resummation has been given in Section III; the magnitude of the NNNLO contribution is sufficiently large to explain the data. Even though we need more accurate data to confirm the theoretical results, this application of the PMC shows the importance of a correct renormalization scale setting for a reliable pQCD prediction.

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