Renormalization group improved pQCD prediction for $\Upsilon(1S)$ leptonic decay

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The complete next-to-next-to-next-to-leading order short-distance and bound-state QCD corrections to $\Upsilon(1S)$ leptonic decay rate $\Gamma(\Upsilon(1S) \to e^+e^-)$ has been finished by Beneke et al. [6]. Based on those improvements, we present a renormalization group (RG) improved pQCD prediction for $\Gamma(\Upsilon(1S) \to e^+e^-)$ by applying the principle of maximum conformality (PMC). The PMC is based on RG-invariance and is designed to solve the pQCD renormalization scheme and scale ambiguities. After applying the PMC for $\Upsilon(1S)$ leptonic decay, all known-type of $\beta$-terms at all orders, which are controlled by the RG-equation, are resummed to determine optimal renormalization scales for its strong running coupling at each order. We then achieve a more convergent pQCD series, a scheme-independent and more accurate pQCD prediction, i.e. $\Gamma_{\Upsilon(1S)\to e^+e^-}|_{\text{PMC}} = 1.361^{+0.124}_{-0.214}$ keV, where the uncertainty is squared average of the mentioned pQCD error sources. This RG-improved pQCD prediction agrees well with the experimental measurement within errors.

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I. INTRODUCTION

Heavy quarkonium provides an ideal platform for studying non-relativistic theories, such as the non-relativistic Quantum Chromodynamics (NRQCD) [1] and the potential NRQCD (PNRQCD) [2]. In general, because $v_b^2 < v^2$ and $\alpha_s(m_b) < \alpha_s(m_c)$, the perturbative results for the bottomonium will be more convergence over the $\alpha_s$- and $v^2$- expansion than the charmonium cases, where $v(b,c)$ stands for the relative velocity of constituent $b$ or $c$ quark in the bottomonium or charmonium rest frame. If enough bottomonium events can be generated at an experimental platform, we can achieve a relatively more definite test of those non-relativistic theories than the charmonium cases.

Being an important high-energy process, the leptonic decay of the ground-state bottomonium $\Upsilon(1S)$ has been studied up to next-to-leading order (NLO) [3, 4], next-to-next-to-leading order (N$^2$LO) [5], and next-to-next-to-next-to-leading order (N$^3$LO) [6]. However, even by including the recently finished complete N$^3$LO QCD corrections for both the short-distance and the bound-state parts, the pQCD prediction for the decay rate $\Gamma_{\Upsilon(1S)\to e^+e^-}$ is still about 30% lower than the PDG value, i.e. $\Gamma_{\Upsilon(1S)\to e^+e^-}|_{\text{Exp}} = 1.340(18)$ keV [6]. Even worse, its pQCD convergence is questionable and one does not know what's the optimal behavior of the running coupling. It is noted that the questionable pQCD series is caused by using conventional scale setting, in which the renormalization scale is simply fixed to be $\sim 3.5$ GeV that leads to maximum decay rate and the renormalization scale uncertainty is predicted by varying it within the range $\mu_r \in [3, 10]$ GeV [6]. To solve such renormalization scale ambiguity and to improve the pQCD prediction, we shall use the principle of maximum conformality (PMC) [8, 10] to deal with $\Upsilon(1S)$ leptonic decay rate up to N$^3$LO level.

The PMC provides a systematic procedure to set the optimal renormalization scale for high-energy processes at any order. The behavior of the running coupling is governed by renormalization group (RG)-equation, i.e. the $\beta$-function [12, 13]

$$\beta(a_s) = \frac{da_s}{d\ln\mu^2} = -a_s^2(\mu_r) \sum_{i=0}^{\infty} \beta_i a_i^i(\mu_r),$$

where $a_s = \alpha_s/4\pi$ and $\mu_r$ is the renormalization scale. This provides the underlying principle of PMC, i.e. the optimal behavior of running coupling can be achieved by resumming all the $\{\beta_i\}$-terms of the process that correctly determine the $\alpha_s$-running behavior into the coupling constant. Following the PMC $R_\Delta$-scheme, the $\beta$-pattern at each perturbative order is a superposition of the $\{\beta_i\}$-terms coming from all the lower-order $\alpha_s$-factors [10]. The PMC then resums the $\{\beta_i\}$-series according to the skeleton-like expansion that correctly reproduces the QED limit of the observable [14]. The resultant PMC scales are functions of the running coupling and are in general different for different orders [17], and the resultant pQCD series is thus identical to a scheme-independent $\beta = 0$ conformal series [8, 10]. Due to the elimination of the $\{\beta_i\}$-terms, the divergent renormalon terms $\beta^n a^n$ disappear accordingly, and the pQCD convergence can be greatly improved. It has been found that the PMC follows the RG-invariance and satisfies all the RG-properties [18]. In the paper, we shall show that after applying the PMC, a more accurate $\Upsilon(1S)$ leptonic decay rate can indeed be achieved.

The remaining parts of the paper are organized as follows. In Sec.II, we will present our calculation technology for the $\Upsilon(1S)$ leptonic decay rate up to N$^3$LO level. In Sec.III, we present numerical results. Sec.IV is reserved for a summary and conclusions. One appendix provide some computational details for PMC.
II. CALCULATION TECHNOLOGY

The decay rate for the channel, $\Upsilon(1S) \to \ell^+\ell^-$, can be formulated as

$$\Gamma_{\Upsilon(1S) \to \ell^+\ell^-} = \frac{4\pi\alpha^2}{9m_b^3} Z_1,$$

where $\alpha$ is the fine structure constant, $m_b$ is the $b$-quark pole mass, and $Z_1$ stands for the residue of the 1S-wave two-point correlation function near (b$b$)-threshold, which can be written as $[13]$

$$Z_1 = |\psi_1(0)|^2 c_v \left[ c_v - \frac{E_1}{m_b} \left( c_v + \frac{d_v}{3} \right) + \cdots \right],$$

where $c_v$ and $d_v$ are matching coefficients of the leading and sub-leading (b$b$)-currents within the NRQCD framework, whose perturbative forms are

$$c_v = 1 + \sum_{k=1}^n c_k a_k^v, \quad d_v = 1 + \sum_{k=1}^n d_k a_k^v,$$

where $a_s = \alpha_s/4\pi$. Here $|\psi_1(0)|$ and $E_1$ are renormalized wavefunction at the origin and binding energy of $\Upsilon(1S)$, which represent the bound-state contributions and also receive perturbative corrections from high-order heavy quark potentials and dynamical gluon effect, i.e.

$$E_1 = E_1^{(0)} \left( 1 + \sum_{k=1}^n e_k a_k^c \right),$$

$$|\psi_1(0)|^2 = |\psi_1^{(0)}(0)|^2 \left( 1 + \sum_{k=1}^n f_k a_k^c \right).$$

The LO Coulomb wavefunction at the origin and the LO Coulomb binding energy are given by $[24, 25]$

$$|\psi_1^{(0)}(0)|^2 = \frac{(m_b C_F \alpha_s)^2}{8\pi},$$

$$E_1^{(0)} = -\frac{1}{2} m_b (C_F \alpha_s)^2,$$

where $C_F = 4/3$. As a further step, those perturbative coefficients $e_i$ and $f_i$ can be separated as

$$e_i = e_i^C + e_i^{nC} + e_i^{us}, \quad f_i = f_i^C + f_i^{nC} + f_i^{us},$$

where ‘C’, ‘nC’ and ‘us’ denote the corrections from the Coulomb potential, all other non-Coulomb potentials and ultrasoft gluon exchange, respectively. The one-loop and two-loop corrections for the Wilson coefficient $c_v$ have been given by Refs. $[24, 25]$. The fermionic and the purely gluonic three-loop corrections to $c_v$ can be found in Refs. $[26, 27]$. The one-loop correction for $d_v$ can be obtained from Ref. $[28]$. For the bound state contributions, its NLO term is from the Coulomb potential, and the ultrasoft correction appears first at the third order. Thus, we have $e_1^{nC} = e_1^{us} = 0$ and $f_1^{nC} = f_1^{us} = 0$. The Coulomb, non-Coulomb and ultrasoft corrections to $E_1$ and $|\psi_1(0)|^2$ have been calculated up to N$^3$LO level in Refs. $[19, 24, 30]$. Up to N$^3$LO level, one can reformulate the pQCD approximate of the decay rate $\Gamma_{\Upsilon(1S) \to \ell^+\ell^-}$ in a perturbative series as

$$\Gamma_n = \sum_{i=0}^{n} C_i a_i^{i+3}(\mu_r).$$

The LO $C_0$ can be derived from Eqs. $[29, 30]$, and $C_i (i \geq 1)$ at each order is a combination of the coefficients $c_k$, $d_k$, $e_k$ and $f_k$ at different orders. There are three energy regions for $\Upsilon(1S)$ leptonic decay, which are characterized by three typical scales, i.e. the hard one $\mu_h \sim m_b$, the soft one $\mu_s \sim m_b v_b$ and the ultra-soft one $\mu_{ul} \sim m_b v_b^2$. Because $v_b \sim \alpha_s(m_b v_b)$, the soft scale $m_b v_b$ is usually replaced by $m_b C_F \alpha_s$, which is the characteristic scale of bottomonium and is connected to its Bohr radius, $r_{Bohr} = 2/(m_b C_F \alpha_s)$.

Under the conventional scale setting, i.e. the renormalization scale is fixed to be its initial value ($\mu_r = \mu_{\text{init}}$) that is usually choose as the typical momentum of the process, the short-distance and bound-state corrections possess both renormalization and factorization scale ambiguities due to the truncation of perturbative series. The factorization scale problem is another important QCD problem, especially for the present case with several energy scales $[17]$. It has been noted that a proper choice of renormalization scale can lead to a smaller factorization scale ambiguity and shall take the same choices for factorization scales in different energy regions as those suggested in the literature, that is, we fix the factorization scales as: $\mu_h = m_b$, $\mu_s = m_b C_F \alpha_s(\mu_s)$ and $\mu_{ul} = m_b C_F \alpha_s^2(\mu_s)$ $[19, 24, 25, 26, 30, 32, 33]$. We note that there exist logarithmic corrections such as the double-logarithmic $\ln^2 \alpha_s$-terms $[36, 37]$ and the single-logarithmic $\ln \alpha_s$-terms $[38, 39]$ in the perturbative bound-state contributions. The origin of those logarithmic corrections is the presence of several scales in the threshold region. They represent a logarithm of the ratio of scales, e.g. a ratio of the hard scale ($m_b$) to the soft one ($m_b v_b$); the resultant $\ln v_b$ equals $\ln \alpha_s$ for bound states that are approximately Coulombic, $v_b \propto \alpha_s$. $[38]$. These corrections are not generated by the renormalization group but are related to the anomalous dimensions of the operators in the effective Hamiltonian $[4]$. Thus in the following PMC treatments, the value of $\ln(\alpha_s)$ is fixed and treated as conformal coefficients, e.g. $\ln(\alpha_s) = \ln(\alpha_s(\mu_s)) \approx -1.1782$.

With all the known results, we are ready to do a PMC analysis of the $\Upsilon(1S)$ leptonic decay rate up to N$^3$LO level. Practically, one can adopt any value $\mu_{\text{init}}$ as the initial renormalization scale to do the renormalization, whose value should be large enough to ensure the pQCD calculation. The three-loop $\Gamma_3$ can be written as

$$\Gamma_3 = c_{1,0} a_3^2(\mu_r^{\text{init}}) + (c_{2,0} + c_{2,1} n_f) a_3^2(\mu_r^{\text{init}})$$
The coefficients $c_{i,j}$ $(i > j \geq 0)$ can be obtained from Refs. [10, 24, 26, 31]. In those references, the coefficients are usually given by setting the factorization scales to be equal to the renormalization scale and by setting the renormalization scale as $m_b$. Thus before applying the PMC, one should first reconstruct all the coefficients with full factorization and renormalization scale dependence. This goal is achieved by using the scale displacement relation derived from the RG-equation [1]. That is, for the coupling $a_s^k(\mu_1)$ at $k_\text{th}$-order, it can be related to the coupling at any other scale $\mu_2$ as

$$a_s^k(\mu_1) = a_s^k(\mu_2) + k \beta_0 \ln \frac{\mu_2^2}{\mu_1^2} a_s^{k+1}(\mu_2) + k \left( \beta_1 \ln \frac{\mu_2^2}{\mu_1^2} + \frac{k+1}{2} \beta_2^2 \ln^2 \frac{\mu_2^2}{\mu_1^2} \right) a_s^{k+2}(\mu_2) + k \left[ \beta_2 \ln \frac{\mu_2^2}{\mu_1^2} + \frac{2k+3}{2} \beta_0 \beta_1 \ln^2 \frac{\mu_2^2}{\mu_1^2} + \frac{(k+1)(k+2)}{3!} \beta_3^3 \ln^3 \frac{\mu_2^2}{\mu_1^2} \right] a_s^{k+3}(\mu_2) + O[a_s^{k+4}(\mu_2)].$$

The derived coefficients $c_{i,j}$ $(i > j \geq 0)$ with full factorization and renormalization scale dependence are put in the Appendix. As a check of our expressions for $c_{i,j}$, we recover the Eq.(3) of Ref. [6] by taking their choices of $\mu_r \equiv \mu_r^{\text{init}}$, $\mu_f = \mu_r$ ($\mu_f = \mu_h, \mu_s, \mu_{us}$) and $n_f = 4$, and by rewriting $[\ln(\mu_r/\mu_0)]$ as $[\ln(\mu_r/m_b) + \ln(\mu_r/\mu_0) + \ln a_s(\mu_r)]$. Furthermore, by setting $\mu_r = m_b$, the three-loop $\Gamma_3$ can be simplified as

$$\Gamma_3 = 0.0734844 a_s^3(m_b) + (2.94406 - 0.380324 n_f) a_s^4(m_b) + (354.456 - 40.8399 n_f + 1.4422 n_f^2) a_s^5(m_b) + (12053.3 - 3286.44 n_f + 226.028 n_f^2 - 4.16436 n_f^3) a_s^6(m_b).$$

Following the standard PMC procedures as shown in Ref. [10], we can obtain the required $\{\beta_i\}$-series at each order from Eq. (11), i.e.

$$\Gamma_3 = r_{1,0} a_s^3(\mu_r^{\text{init}}) + (r_{2,0} + 3 \beta_0 r_{2,1}) a_s^4(\mu_r^{\text{init}}) + (r_{3,0} + 3 \beta_1 r_{2,1} + 4 \beta_0 r_{3,1} + 6 \beta_0^2 r_{3,2}) a_s^5(\mu_r^{\text{init}}) + (r_{4,0} + 3 \beta_2 r_{2,1} + 4 \beta_1 r_{3,1} + 5 \beta_0 r_{4,1} + \frac{27}{2} \beta_1 \beta_0 r_{3,2} + 10 \beta_2^2 r_{4,2} + 10 \beta_0^3 r_{4,3}) a_s^6(\mu_r^{\text{init}}).$$

The $\beta_i$ coefficients $r_{i,j}$ $(i > j \geq 0)$ can be obtained from the $n_f$ coefficients $c_{i,j}$ $(i > j \geq 0)$ by applying basic PMC formulas listed in Ref. [10]. The non-conformal coefficients $r_{i,j}$ $(j \neq 0)$ are functions of $\mu_r^{\text{init}}$; while, the conformal coefficients $r_{i,0}$ are independent of $\mu_r^{\text{init}}$. For convenience, we present the conformal coefficients $r_{i,0}$ with explicit factorization scale and/or initial scale dependence in the Appendix.

After applying the PMC, the three-loop leptonic decay rate $\Gamma(1S)$ changes to

$$\Gamma_3 = r_{1,0} a_s^3(Q_1) + r_{2,0} a_s^4(Q_2) + r_{3,0} a_s^5(Q_3) + r_{4,0} a_s^6(Q_4),$$

where $Q_i (i = 1, 2, 3, 4)$ are PMC scales at each perturbative order, whose expressions with explicit factorization scale and/or initial scale dependence are put in the Appendix. To eliminate the non-conformal $\beta$-terms, the renormalization scales at each perturbative order have been shifted from its initial value $\mu_r^{\text{init}}$ to the optimal ones $Q_i$ at different orders. The PMC scales at each order are determined unambiguously by resuming all the $Q_i$-terms, we cannot determine $Q_4$, and we simply set $Q_4 = Q_3$ in the following calculation. This treatment will lead to residual scale dependence, which, however, will be highly suppressed [17].
III. NUMERICAL RESULTS

We adopt four-loop $\alpha_s$-running to do the numerical analysis of the three-loop $\Upsilon(1S)$ leptonic decay rate. By taking $\alpha_s(M_Z) = 0.1185$, we obtain $\Lambda_{\text{QCD}}^{(n_f=3)} = 0.349 \text{ GeV}$, $\Lambda_{\text{QCD}}^{(n_f=4)} = 0.301 \text{ GeV}$, and $\Lambda_{\text{QCD}}^{(n_f=5)} = 0.214 \text{ GeV}$. We take the fine structure constant $\alpha(2m_b) = 1/132.3$. Using the highest known three-loop relation between the pole mass and MS-running mass and taking the $b$-quark MS-mass $m_b(m_b) = 4.18 \text{ GeV}$, we obtain the $b$-quark pole mass $m_b = 4.92 \text{ GeV}$.

We first present the decay rate $\Gamma_{\Upsilon(1S)\to \ell^+\ell^-}$ with different loop corrections in Fig. 1, in which the conventional scale setting method with the renormalization scale $\mu_r \equiv \mu_r^{\text{init}}$ is adopted. To be self-consistent, when calculating $\Gamma_n$, the $(n+1)$th-loop $\alpha_s$-running together with its own $\Lambda_{\text{QCD}}$ value are adopted. Fig. 1 agrees with the conventional wisdom that with the increment of loop corrections, the conventional scale dependence becomes smaller. It also indicates that the higher-order terms are important for an accurate pQCD prediction.

In Fig. 2, we present the initial scale dependence for the PMC scales $Q_1$, $Q_2$ and $Q_3$. Fig. 2 shows that the PMC scales $Q_i$ are almost independent on the choice of initial renormalization scale $\mu_r^{\text{init}}$ by varying it within a large perturbative region such as $2 \sim 20 \text{ GeV}$. If setting $\mu_r^{\text{init}} = m_b$, we find the LO PMC scale $Q_1 \simeq 1.31 \text{ GeV}$, the NLO PMC scale $Q_2 \simeq 2.02 \text{ GeV}$ and the $N^2\text{LO}$ PMC scale $Q_3 \simeq 5.10 \text{ GeV}$. Those scales are different from the guessed value $\sim 3.5 \text{ GeV}$ that leads to maximum decay rate under conventional scale setting.

| LO   | NLO  | $N^2\text{LO}$ | $N^3\text{LO}$ | sum   |
|------|------|----------------|----------------|-------|
| Conv. | +0.374 | +0.125 | +0.322 | +0.061 | +0.882 |
| PMC  | +2.382 | -1.198 | +0.192 | -0.015 | +1.361 |

TABLE I. Contributions from each order for the three-loop decay rate $\Gamma_3$ (in unit: keV) under the conventional (Conv.) and the PMC scale settings, respectively. $\mu_r^{\text{init}} = m_b$.

| $K_1$ | $K_2$ | $K_3$ |
|-------|-------|-------|
| Conv. | 33.4% | 64.5% | 7.4% |
| PMC   | 50.3% | 16.2% | 1.1% |

TABLE II. The defined $K$ factor ($K_n$) for the $N^n\text{LO}$ term of $\Gamma_3$ before and after the PMC scale setting, where $n = 1$, 2 and 3, respectively. $\mu_r^{\text{init}} = m_b$.

The non-conformal terms determine the renormalization scales at each perturbative order and the conformal terms as well as the resultant PMC scales accurately display the magnitude of the pQCD correction at each perturbative order. After applying the PMC, the pQCD convergence can be improved due to the elimination of divergent renormalon terms. For example, we present the contributions from each order for $\Gamma_3$ in Table II, in which the results before and after the PMC scale setting are presented. Under conventional scale setting, the $N^2\text{LO}$ term is about 90% of the LO term, and is almost three times of the NLO term, breaking the pQCD nature of the series. After applying the PMC, the pQCD convergence is improved, the magnitude of $N^2\text{LO}$ term is about 16% of the NLO term and the magnitude of $N^3\text{LO}$ term is about 8% of the $N^2\text{LO}$ term. This can be show more clearly by defining a $K$ factor ($K_n$) that equals to the

\footnote{The choice of $b$-quark pole mass and also $|\psi_1^{(0)}(0)|^2$ and $E_1^{(0)}$ in final expresses ensure the correct using of PMC, since only those $\beta$-terms that are pertained to the renormalization of the running coupling should be absorbed into the running coupling. Here we also do not consider the non-perturbative corrections/uncertainties for $|\psi_1^{(0)}(0)|$ and $E_1^{(0)}$.}
magnitude of the ratio between the $n_{th}$-order term and the sum of all lower-order terms. The $K$ factors for NLO, N$^2$LO and N$^3$LO terms are presented in Table II.

In Fig. 3, we present the three-loop $\Gamma_3$ versus the choice of initial scale $\mu_{\text{init}}$, in which the results before and after the PMC scale setting are presented as a comparison. Under conventional scale setting, the decay rate $\Gamma_3$ shall first increase and then decrease with the increment of $\mu_{\text{init}}$; If setting $\mu_{\text{init}} = \mu_{\text{init}} \sim 3.5$ GeV, we obtain its maximum value, which however is still lower than the central PDG value by about 30%. After applying the PMC, the decay rate $\Gamma_3$ monotonously raises with the increment of $\mu_{\text{init}}$, and the renormalization scale dependence has been greatly suppressed. By taking a hard enough scale such as $\mu_{\text{init}} > 4$ GeV, the computed PMC scales and the final PMC prediction for the leptonic $\Upsilon(1S)$ decay are highly independent to its exact values. If taking $\mu_{\text{init}} = m_0$, we obtain

$$\Gamma_{\Upsilon(1S) \to e^+e^-} = 1.361 \text{ keV},$$  
(15)

which agrees with the central PDG value within 2% error [7].

For the present process, the perturbative series starts at $\alpha_s^3$, slight change of its argument shall result in large pQCD error, thus this process provides a good platform for testing the correct running behavior of the coupling constant. On the one hand, the PMC prediction for $\Upsilon(1S)$ leptonic decay reads

$$\Gamma_{\Upsilon(1S) \to e^+e^-} |_{\text{PMC}} = 1.361^{+0.147+0.042}_{-0.209-0.041} \pm 0.015 \text{ keV} \text{(16)}$$

$$= 1.361^{+0.154}_{-0.214} \text{ keV},$$  
(17)

where the first error is the residual initial scale dependence for $\mu_{\text{init}} \in \{3, 10\}$ GeV, the second error is for $\alpha_s(M_Z)_{\text{Exp.}} = 0.1185 \pm 0.0006$ [2], and the third error is the estimated unknown higher-order contributions. The errors in the second line stand for the squared averages of those errors. The unknown higher-order contribution is predicted as $|C_3a_s^{\text{MAX}}| [1]$, where the symbol

"MAX" stands for the maximum $|C_3a_s^{\text{MAX}}| within the region of $\mu_{\text{init}} \in \{3, 10\}$ GeV. This RG-improved pQCD prediction agrees well with the experimental measurement. It is noted that for the present case, even though the PMC scales themselves are almost flat within the region of $\mu_{\text{init}} \in \{3, 10\}$ GeV, cf. Fig. 2, there is large residual scale dependence in comparison to the previous PMC examples, such as Refs. [11][14]. Thus we need to know even higher-order $\beta$-terms for this particular process so as to achieve accurate PMC scales and PMC predictions.

On the other hand, the present PMC prediction on the $\Upsilon(1S)$ decay rate together with its errors can be compared with the prediction under the conventional scale setting

$$\Gamma_{\Upsilon(1S) \to e^+e^-} |_{\text{Conv.}} = 0.882^{+0.022+0.023}_{-0.120-0.022} \pm 0.443 \text{ keV} \text{(18)}$$

$$= 0.882^{+0.444}_{-0.459} \text{ keV},$$  
(19)

where the first error is initial scale dependence for $\mu_{\text{init}} \in \{3, 10\}$ GeV, the second error is from $\alpha_s(M_Z)_{\text{Exp.}}$ uncertainty, and the third error is the estimated unknown higher-order contributions. The errors in the second line stand for the squared averages of those errors. The central decay rate is lower than the central PDG value by about 34%, and the much larger errors in comparison to the PMC prediction are caused by the large value of N$^3$LO term at the scale 3 GeV, which are consistent with observation shown in Ref. [6].

IV. SUMMARY

We have studied the N$^3$LO short-distance and bound-state QCD corrections to $\Upsilon(1S)$ leptonic decay rate of $\Upsilon(1S) \to \ell^+\ell^-$ by applying the PMC. A comparison of the three-loop $\Gamma_3$ together with its pQCD errors before and after the PMC scale setting is presented in

FIG. 3. The $\Gamma_3$ versus the initial renormalization scale $\mu_{\text{init}}$ before and after the PMC scale setting. The dashed and solid lines are for the conventional (Conv.) and the PMC scale settings, respectively.

FIG. 4. A comparison of $\Gamma_3$ together with its pQCD errors before and after the PMC scale setting. The theoretical errors are squared average of all the mentioned uncertainties. The PDG value, $\Gamma_{\Upsilon(1S) \to e^+e^-} |_{\text{Exp.}} = 1.340(18) \text{ keV}$ [2], is included as a comparison.
where the theoretical errors are squared averages of all the mentioned pQCD uncertainties. With higher-order renormalon terms being resummed into the running coupling, the pQCD convergence of the resultant series are improved. Thus, the PMC does provide a systematic and unambiguous way to set the renormalization scale for any QCD processes and the accuracy of the pQCD prediction can be greatly improved. It is noted that we have not considered the non-perturbative corrections/uncertainties for $|\psi_1(0)|$ and $E_1$, and for the decay rate $\Gamma(\Upsilon(1S) \to \ell^+\ell^-\gamma)$. Those studies shall further improve our present PMC predictions, which are out of the range of the present paper.

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Appendix A: The conformal coefficients and the PMC scales for $\Gamma_3$

In this Appendix, we first present the coefficients $c_{i,j}$ for $n_f$-power series, and then present the conformal coefficients $r_{i,0}$ and the PMC scales $Q_i$ for the three-loop $\Upsilon(1S)$ leptonic decay rate $\Gamma_3$. The full renormalization scale and factorization scale dependence have been explicitly presented.

As mentioned in the body of the text, the coefficients $c_{i,j}$ ($i > j \geq 0$) for $n_f$-power series can be derived by using the scale displacement relation (12) from those of Refs. [19, 27, 29, 30], which are

\begin{align}
c_{1,0} &= 0.0734844, \\
c_{2,0} &= -1.37493 + 4.84997L(\mu_{r}^{\text{init}}), \\
c_{2,1} &= -0.118568 - 0.293938L(\mu_{r}^{\text{init}}), \\
c_{3,0} &= 168.629 - 41.5323L(\mu_{r}^{\text{init}}) + 213.399L^2(\mu_{r}^{\text{init}}) + 60.1699L(\mu_b) - 106.699L(\mu_s) \\
&= 34.4887 \ln \frac{\mu_{b}^{\text{init}}}{m_b} - 60.1699 \ln \frac{\mu_{b}}{m_b}, \\
c_{3,1} &= -10.7309 - 10.7761L(\mu_{r}^{\text{init}}) - 25.8665L^2(\mu_{r}^{\text{init}}) + 12.9333L(\mu_s) + 2.09022 \ln \frac{\mu_{b}^{\text{init}}}{m_b}, \\
c_{3,2} &= 0.257472 + 0.632361L(\mu_{r}^{\text{init}}) + 0.783834L^2(\mu_{r}^{\text{init}}) - 0.391917L(\mu_s), \\
c_{4,0} &= -14311.9 - 1283.62L(\mu_b) + 22709.0L(\mu_{r}^{\text{init}}) + 6618.69L(\mu_b)L(\mu_{r}^{\text{init}}) + 832.64L^2(\mu_{r}^{\text{init}}) \\
&\quad + 7824.62L^3(\mu_{r}^{\text{init}}) + 8857.05L(\mu_s) - 6618.69L(\mu_b)L(\mu_s) - 11736.9L(\mu_{r}^{\text{init}})L(\mu_s) \\
&\quad + 8102.97L^2(\mu_s) + 939.94L(\mu_{s}^{\text{init}}) + 518.834 \ln \frac{\mu_{b}}{m_b} - 3971.21L(\mu_{r}^{\text{init}}) \ln \frac{\mu_{b}^{\text{init}}}{m_b} \\
&\quad + 160.453L(\mu_{s}^{\text{init}}) \ln \frac{\mu_{b}^{\text{init}}}{m_b} + 40.1133L^2(\mu_{b}^{\text{init}}) - 4651.9 \ln \frac{\mu_{b}^{\text{init}}}{m_b} - 2276.25L(\mu_{r}^{\text{init}}) \ln \frac{\mu_{b}^{\text{init}}}{m_b} \\
&\quad - 2647.48 \ln \frac{\mu_{b}^{\text{init}}}{m_b} \ln \frac{\mu_{r}^{\text{init}}}{m_b} - 758.751L^2(\mu_{r}^{\text{init}}) - 7097.75 \ln \frac{\mu_{b}^{\text{init}}}{m_b} - 511.158 \ln^2 \frac{\mu_{s}^{\text{init}}}{m_b} \\
&\quad + 7586.97 \ln \alpha_s(\mu_s) + 3429.11 \ln \frac{\mu_b}{m_b} \ln \alpha_s(\mu_s) - 2727.7 \ln^2 \alpha_s(\mu_s), \\
c_{4,1} &= 1458.98 - 2785.37L(\mu_{r}^{\text{init}}) - 401.133L(\mu_b)L(\mu_{r}^{\text{init}}) - 957.856L^2(\mu_{r}^{\text{init}}) - 1422.66L^3(\mu_{r}^{\text{init}}) \\
&\quad - 212.745L(\mu_s) + 401.133L(\mu_b)L(\mu_s) + 2133.99L(\mu_{r}^{\text{init}})L(\mu_s) - 534.305L^2(\mu_s) \\
&\quad + 97.0847 \ln \frac{\mu_{b}^{\text{init}}}{m_b} + 240.68L(\mu_{r}^{\text{init}}) \ln \frac{\mu_{b}^{\text{init}}}{m_b} + 400.066 \ln \frac{\mu_{r}^{\text{init}}}{m_b} + 275.909L(\mu_{r}^{\text{init}}) \ln \frac{\mu_{b}^{\text{init}}}{m_b} \\
&\quad + 160.453 \ln \frac{\mu_{b}^{\text{init}}}{m_b} \ln \frac{\mu_{r}^{\text{init}}}{m_b} + 91.9698 \ln^2 \frac{\mu_{r}^{\text{init}}}{m_b} + 133.615 \ln \frac{\mu_{s}^{\text{init}}}{m_b} - 80.2265 \ln^2 \frac{\mu_{s}^{\text{init}}}{m_b}, \\
c_{4,2} &= -13.3227 + 120.457L(\mu_{r}^{\text{init}}) + 89.7734L^2(\mu_{r}^{\text{init}}) + 86.2217L^3(\mu_{r}^{\text{init}}) - 9.85995L(\mu_s) \\
&\quad - 129.333L(\mu_{r}^{\text{init}})L(\mu_s) + 12.9333L^2(\mu_s) - 5.92731 \ln \frac{\mu_{r}^{\text{init}}}{m_b} - 8.36089L(\mu_{r}^{\text{init}}) \ln \frac{\mu_{r}^{\text{init}}}{m_b} \\
&\quad - 2.78696 \ln^2 \frac{\mu_{r}^{\text{init}}}{m_b}, \\
c_{4,3} &= 0.265871 - 1.71648L(\mu_{r}^{\text{init}}) - 2.10787L^2(\mu_{r}^{\text{init}}) - 1.74185L^3(\mu_{r}^{\text{init}}) + 0.320593L(\mu_s) \\
&\quad - 1.66705L(\mu_b)L(\mu_{r}^{\text{init}}) - 0.66705L(\mu_{r}^{\text{init}})L(\mu_s) - 0.66705L^2(\mu_{r}^{\text{init}}) \\
&\quad - 0.66705L^3(\mu_{r}^{\text{init}}) - 0.66705L^4(\mu_{r}^{\text{init}}). 
\end{align}
where $\mu_h$, $\mu_s$ and $\mu_{as}$ stand for the hard, the soft and the ultra-soft factorization scales, respectively. The functions $L(\mu_r^{\text{init}}) = \ln[\mu_r^{\text{init}}/(m_b C_F \alpha_s(\mu_s))]$,

$L(\mu_b) = \ln[\mu_b/(m_b C_F \alpha_s(\mu_s))]$, $L(\mu_s) = \ln[\mu_s/(m_b C_F \alpha_s(\mu_s))]$ and $L(\mu_{as}) = \ln[\mu_{as}/(m_b C_F \alpha_s(\mu_s))]$.

The conformal coefficients $r_{i,0}(i = 1, 2, 3, 4)$ read

$$r_{1,0} = 0.0734844, \quad (A11)$$

$$r_{2,0} = -3.33129, \quad (A12)$$

$$r_{3,0} = 80.6951 + 60.1699 L(\mu_b) - 60.1699 \ln \frac{\mu_h}{m_b}(A13)$$

$$r_{4,0} = 7600.61 - 1283.62 L(\mu_b) + 4102.54 L(\mu_s) + 1634.33 L^2(\mu_s) + 939.94 L(\mu_{as})$$

$$+160.453 L(\mu_s) \ln \frac{\mu_h}{m_b} + 2120.73 \ln \frac{\mu_h}{m_b} + 40.1133 \ln \frac{\mu_h}{m_b} - 4893.09 \ln \frac{\mu_s}{m_b}$$

$$-1834.9 \ln \frac{\mu_s}{m_b} + 7586.97 \ln \alpha_s(\mu_s) + 3429.11 \ln \frac{\mu_s}{m_b} \ln \alpha_s(\mu_s)$$

$$-2727.2 \ln^2 \alpha_s(\mu_s). \quad (A14)$$

As required, these equations show that the conformal coefficients are free of initial scale dependence. The PMC scales $Q_i(i = 1, 2, 3)$ with full initial scale and factorization scale dependence for each perturbative order read

$$\ln \frac{Q_i^2}{(\mu_r^{\text{init}})^2} = -0.806755 - 2 L(\mu_r^{\text{init}}) - \left(1.32611 - 4 L(\mu_s)\right) \beta_0 \alpha_s(\mu_r^{\text{init}}) + a_s^2(\mu_r^{\text{init}}) \left[10.1 - 2.65222 L(\mu_r^{\text{init}})ight.$$}

$$-8 L(\mu_s) + 8(L(\mu_r^{\text{init}}) L(\mu_s) - 4 L^2(\mu_s)) \beta_0^2 - \left(1.65764 - 5 L(\mu_s)\right) \beta_1], \quad (A15)$$

$$\ln \frac{Q_i^2}{(\mu_r^{\text{init}})^2} = -0.0020727 - 1.76471 L(\mu_r^{\text{init}}) - 0.235294 \ln \frac{\mu_r^{\text{init}}}{m_b} + a_s(\mu_r^{\text{init}}) \beta_0 - 2.06665 + 0.998408 L(\mu_r^{\text{init}})$$

$$-0.33218 L^2(\mu_r^{\text{init}}) + 3.84375 L(\mu_s) - \left(0.998408 - 0.66436 L(\mu_r^{\text{init}})\right) \ln \frac{\mu_r^{\text{init}}}{m_b} - 0.33218 \ln^2 \frac{\mu_r^{\text{init}}}{m_b} \quad (A16)$$

$$\ln \frac{Q_i^2}{(\mu_r^{\text{init}})^2} = \left[5.77145 - 3.50367 L(\mu_r^{\text{init}}) - 2 L(\mu_s) L(\mu_r^{\text{init}}) - 0.671837 L(\mu_s) + 2 L(\mu_b) L(\mu_s) - 1.6 L^2(\mu_s)$$

$$+ \left(0.484053 + 1.2 L(\mu_r^{\text{init}}) + 0.8 \ln \frac{\mu_r^{\text{init}}}{m_b}\right) \ln \frac{\mu_h}{m_b} + 0.821428 \ln \frac{\mu_h}{m_b} + 0.66619 \ln \frac{\mu_s}{m_b}$$

$$-0.4 \ln^2 \frac{\mu_s}{m_b}\right]/\left(1.34112 + L(\mu_h) - \ln \frac{\mu_h}{m_b}\right). \quad (A17)$$

As a minor point, we have found that there are some typos for the general coefficients $r_{4,j}$ with $j = (0, 1, 2)$ at the four-loop level, i.e. Eqs.(39b-39d) of Ref.[10] (they are correct for $n = 1$) should be corrected as

$$r_{4,2} = \frac{1}{32(n + 1)(n + 2) T^3} \left[2 T^2 c_{2,1}(79 C_A + 66 C_F) - 9 \left(\frac{4(3 + 2 n)}{n + 1} T c_{3,2}(5 C_A + 3 C_F) - 33 c_{4,3} C_A - 4 T c_{4,2}\right)\right] \quad (A18)$$

$$r_{4,1} = \frac{1}{64(n + 2) T^3} \left[4 T^2 c_{2,1}(-397 C_A C_F - 118 C_A^2 - 126 C_F^2) + 48 T^2 c_{3,1}(5 C_A + 3 C_F)$$

$$+ \frac{12 T c_{3,2}}{n + 1} C_A ((152 n + 173) C_A + 33(4n + 5) C_F) - 33 C_A (33 c_{4,3} C_A + 8 T c_{4,2}) - 48 T^2 c_{4,1}\right], \quad (A19)$$

$$r_{4,0} = c_{4,0} + \frac{1}{64 T^3} \left[2 T^2 c_{2,1} C_A (1208 C_A C_F - 287 C_A^2 + 924 C_F^2) - 48 T^2 c_{3,1} C_A (7 C_A + 11 C_F)$$

$$-2904 T c_{3,2} C_A^2 C_F + 176 T^2 c_{4,1} C_A - 1848 T c_{3,2} C_A^3 + 484 T c_{4,2} C_A^2 + 1331 c_{4,3} C_A^3\right]. \quad (A20)$$
[1] G.T. Bodwin, E. Braaten, and G.P. Lepage, Phys. Rev. D 51, 1125 (1995); 55, 5853(E) (1997).

[2] A. Pineda and J. Soto, Nucl. Phys. B, Proc. Suppl. 64, 428 (1998); N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Nucl. Phys. B 566, 275 (2000).

[3] A. Pineda, Nucl. Phys. B 494, 213 (1997).

[4] A. Pineda, Phys. Rev. D 66, 054022 (2002).

[5] M. Beneke and A. Signer, Phys. Lett. B 471, 233 (1999).

[6] M. Beneke, Y. Kiyo, P. Marquard, A. Penin, J. Piclum, D. Seidel, and M. Steinhauser, Phys. Rev. Lett. 112, 151801 (2014).

[7] K.A. Olive et al., (Particle Data Group), Chin. Phys. C 38, 090001 (2014).

[8] S.J. Brodsky and X.G. Wu, Phys. Rev. D 85, 034038 (2012); Phys. Rev. Lett. 109, 042002 (2012); Phys. Rev. D 85, 114040 (2012); Phys. Rev. D 86, 014021 (2012).

[9] M. Mojaza, S.J. Brodsky, and X.G. Wu, Phys. Rev. Lett. 110, 192001 (2013).

[10] S.J. Brodsky, M. Mojaza, and X.G. Wu, Phys. Rev. D 89, 014027 (2014).

[11] X.G. Wu, S.J. Brodsky, and M. Mojaza, arXiv:1405.3196.

[12] H.D. Politzer, Phys. Rev. Lett. 30, 1346 (1973).

[13] D. Gross and F. Wilczek, Phys. Rev. Lett. 30, 1343 (1973).

[14] H.D. Politzer, Phys. Rept. 14, 129 (1974).

[15] D.J. Gross and F. Wilczek, Phys. Rev. D 8, 3633 (1973); Phys. Rev. D 9, 980 (1973).

[16] S.J. Brodsky and P. Huet, Phys. Lett. B 417, 145 (1998).

[17] X.G. Wu, S.J. Brodsky, and M. Mojaza, Prog. Part. Nucl. Phys. 72, 44 (2013).

[18] S.J. Brodsky and X.G. Wu, Phys. Rev. D 86, 054018 (2012).

[19] M. Beneke, Y. Kiyo, and K. Schuller, Phys. Lett. B 658, 222 (2008).

[20] S. Titard and F.J. Yndurain, Phys. Rev. D 49, 6007 (1994); S. Titard and F.J. Yndurain, Phys. Rev. D 51, 6348 (1995).

[21] B.A. Kniehl and A.A. Penin, Nucl. Phys. B 563, 200 (1999).

[22] K. Melnikov and A. Yelkhovsky, Phys. Rev. D 59, 114009 (1999).

[23] A.A. Penin and A.A. Pivovarov, Nucl. Phys. B 549, 217 (1999).

[24] G. Kallen, A. Sabry, and K. Dan.Vidensk.Selsk., Mat. Fys. Medd. 29, 1 (1955).

[25] A. Czarnecki and K. Melnikov, Phys. Rev. Lett. 80, 2531 (1998); M. Beneke, A. Signer, and V. A. Smirnov, Phys. Rev. Lett. 80, 2535 (1998); B. A. Kniehl, A. Onischenko, J. H. Piclum, and M. Steinhauser, Phys. Lett. B 638, 209 (2006).

[26] P. Marquard, J.H. Piclum, D. Seidel, and M. Steinhauser, Nucl. Phys. B 758, 144 (2006); Phys. Lett. B 678, 269 (2009).

[27] P. Marquard, J.H. Piclum, D. Seidel, and M. Steinhauser, Phys. Rev. D 89, 034027 (2014).

[28] M.E. Luke and M. J. Savage, Phys. Rev. D 57, 413 (1998).

[29] M. Beneke, Y. Kiyo, and K. Schuller, Nucl. Phys. B 714, 67 (2005); A.A. Penin, V.A. Smirnov, and M. Steinhauser, Nucl. Phys. B 716, 303 (2005).

[30] M. Beneke, Y. Kiyo, and A.A. Penin, Phys. Lett. B 653, 53 (2007); M. Beneke and Y. Kiyo, Phys. Lett. B 668, 143 (2008).

[31] S.Q. Wang, X.G. Wu, Z.G. Si, and S.J. Brodsky, Phys. Rev. D 90, 114034 (2014).

[32] M. Beneke and V. A. Smirnov, Nucl. Phys. B 522, 321 (1998).

[33] M. Beneke, A. Signer, and V.A. Smirnov, Phys. Lett. B 454, 137 (1999).

[34] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Rev. Mod. Phys. 77, 1423 (2005).

[35] C. Anzai, Y. Kiyo, and Y. Sumino, Phys. Rev. Lett. 104, 112003 (2010).

[36] B.A. Kniehl and A.A. Penin, Nucl. Phys. B 577, 197 (2000).

[37] A.V. Manohar and I.W. Stewart, Phys. Rev. D 63, 054004 (2001).

[38] B.A. Kniehl, A.A. Penin, V.A. Smirnov, and M. Steinhauser, Phys. Rev. Lett. 90, 212001 (2003); 91, 139903(E) (2003).

[39] A.H. Hoang, Phys. Rev. D 69, 034009 (2004).

[40] F. Jegerlehner, Nuovo Cimento Soc. Ital. Fis. 034S1 (2011) 31.

[41] S.Q. Wang, X.G. Wu, X.C. Zheng, G. Chen, and J.M. Shen, J. Phys. G 41, 075010 (2014).

[42] S.Q. Wang, X.G. Wu, J.M. Shen, H.Y. Han, and Y. Ma, Phys. Rev. D 89, 116001 (2014).

[43] S.Q. Wang, X.G. Wu, and S.J. Brodsky, Phys. Rev. D 90, 037503 (2014).

[44] S.Q. Wang, X.G. Wu, X.C. Zheng, J.M. Shen, and Q.L. Zhang, Eur. Phys. J. C 74, 2825 (2014).