Potential Nonrelativistic QCD and Heavy Quarkonium Spectrum in Next-to-Next-to-Next-to-Leading Order

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In this talk I review the calculation of the third order corrections to the heavy quarkonium spectrum in the nonrelativistic effective theory framework and its application to the phenomenology of top quark threshold production.

1. INTRODUCTION

The theoretical study of the nonrelativistic heavy quark-antiquark system and its application to bottomonium and toponium physics is of special interest because it relies entirely on the first principles of QCD. The system in principle allows for a perturbative treatment with the nonperturbative effects being well under control and with no crucial model dependence. This makes the heavy quarkonium to be an ideal place to determine the fundamental QCD parameters such as the heavy quark mass $m_q$ and the strong coupling constant $\alpha_s$. An essential progress has been made in the theoretical investigation of the nonrelativistic heavy quark dynamics based on the effective theory approach. The analytical results for the main parameters of the nonrelativistic heavy quark-antiquark system are now available up to next-to-next-to-leading order (NNLO) (see for a brief review). The NNLO corrections have turned out to be so sizeable that it appears to be indispensable also to gain control over the next-to-next-to-next-to-leading order (N$^3$LO) both in regard of phenomenological applications and in order to understand the structure and the peculiarities of the nonrelativistic expansion. The calculation of the heavy-quarkonium spectrum to $O(\alpha_s^3)$ was the first breakthrough in the N$^3$LO analysis. Recently, the $O(\alpha_s^3 \ln \alpha_s)$ corrections to the heavy-quarkonium production and annihilation rates have been also obtained. The subject of this talk is restricted mainly to the analysis of the spectrum.

In the next section we briefly introduce the basic ingredients of the nonrelativistic effective-theory formalism. In Sect. 3 the structure of the third order corrections to the heavy quarkonium ground state energy is outlined and the final result is presented. In the last section this result is applied for the phenomenological analysis of the top-antitop pair production near the threshold.

2. EFFECTIVE THEORY OF NONRELATIVISTIC HEAVY QUARKS

The nonrelativistic behavior of the heavy-quark-antiquark pair is governed by a complicated multiscale dynamics. In the nonrelativistic regime, where the heavy-quark velocity $v$ is of the order of the strong-coupling constant $\alpha_s$, the Coulomb effects are crucial and have to be taken into account to all orders in $\alpha_s$. This makes the use of the effective theory mandatory. The effective-theory approach allows us to separate the scales and to implement the expansion in $v$ at the level of the Lagrangian. Let us recall that the dynamics of a nonrelativistic quark-antiquark pair is characterized by four different regions and the corresponding modes: (i) the hard region (the energy and three-momentum scale like $m_q$); (ii) the soft region (the energy and three-momentum scale like $m_q v$); (iii) the potential re-
region (the energy scales like \( m_q v^2 \), while the three-momentum scales like \( m_q v \)); and (iv) the ultrasoft region (the energy and three-momentum scale like \( m_q v^2 \)). Nonrelativistic QCD (NRQCD) \( [4] \) is obtained by integrating out the hard modes. Subsequently integrating out the soft modes and the potential gluons results in the effective theory of potential NRQCD (pNRQCD) \( [10] \), which contains potential heavy quarks and ultrasoft gluons, ghosts, and light quarks as active particles. The effect of the modes that have been integrated out is two-fold: higher-dimensional operators appear in the effective Hamiltonian, corresponding to an expansion in \( v \), and the Wilson coefficients of the operators in the effective Hamiltonian acquire corrections, which are series in \( \alpha_s \).

The theory of pNRQCD is relevant for the description of the heavy-quarkonium system. Let us recall its basic ingredients. In pNRQCD, the (self)interactions between ultrasoft particles are described by the standard QCD Lagrangian. The interactions of the ultrasoft gluons with the heavy-quark-antiquark pair are ordered in \( v \) by the multipole expansion. For the N^3LO analysis, only the leading-order (LO) emission and absorption of ultrasoft gluons have to be considered. They are described by the chromoelectric dipole interaction. The propagation of the quark-antiquark pair in the colour-singlet and colour-octet states is described by the nonrelativistic Green function of the effective Schrödinger equation. The LO approximation for the Green function is given by the Coulomb solution, which sums up terms singular at threshold and describes the leading binding effects. The corrections due to higher-order terms in the effective Hamiltonian can be found in Rayleigh-Schrödinger time-independent perturbation theory as in standard quantum mechanics.

Let us now turn to the problem of perturbative calculations in the effective theory. Both NRQCD and pNRQCD have specific Feynman rules, which can be used for a systematic perturbative expansion. However, this is complicated because the expansion of the Lagrangian corresponds to a particular subspace of the total phase space. Thus, in a perturbative calculation within the effective theory, one has to formally impose some restrictions on the allowed values of the virtual momenta. Explicitly separating the phase space introduces additional scales to the problem, such as momentum cutoffs, and makes the approach considerably less transparent. A much more efficient and elegant method is based on the expansion by regions \( [9] \), which is a systematic method to expand Feynman diagrams in any limit of momenta and masses. It consists of the following steps: (i) consider various regions of a loop four-momentum \( k \) and expand, in every region, the integrand in Taylor series with respect to the parameters that are considered to be small there; (ii) integrate the expanded integrand over the whole integration domain of the loop momenta; and (iii) put to zero any scaleless integral. In step (ii), dimensional regularization, with \( d = 4 - 2\epsilon \) space-time dimensions, is used to handle the divergences. In the case of the threshold expansion in \( v \), one has to deal with the four regions and their scaling rules listed above. In principle, the threshold expansion has to be applied to the Feynman diagrams of full QCD. However, after integrating out the hard modes, which corresponds to calculating the hard-region contributions in the threshold expansion, it is possible to apply step (i) to the diagrams constructed from the NRQCD and pNRQCD Feynman rules. Equivalently, the Lagrangian of the effective theory can be employed for a perturbative calculation without explicit restrictions on the virtual momenta if dimensional regularization is used and the formal expressions derived from the Feynman rules of the effective theory are understood in the sense of the threshold expansion. In this way, one arrives at a formulation of effective theory with two crucial virtues: the absence of additional regulator scales and the automatic matching of the contributions from different scales \( [9,11] \) (see also \( [12] \)). The second property implies that the contributions of different modes, as computed in the effective theory, can be simply added up to get the full result.

### 3. Heavy Quarkonium Spectrum at \( \mathcal{O}(\alpha_s^5 m_q) \)

The analysis of the heavy quarkonium spectrum at \( \mathcal{O}(\alpha_s^5 m_q) \) i.e. the third order correc-
tions to the Coulomb approximation involves two basic ingredients: the effective Hamiltonian and the retardation effect associated with the emission and absorption of dynamical ultrasoft gluons. The general form of the Hamiltonian valid up to NextLO is given in \( \text{Ref.} 1 \). A detailed discussion of the effects resulting from the chromoelectric dipole interaction of the heavy quark-antiquark pair to the ultrasoft gluons relevant for perturbative bound-state calculations at NextLO can be found in \( \text{Ref.} 1 \).

For vanishing angular momentum we can write the energy level of the principal quantum number \( n \) as

\[
E_n^{\text{p+1}} = E_n^C + \delta E_n^{(1)} + \delta E_n^{(2)} + \delta E_n^{(3)} + \ldots ,
\]

(1)

where the leading order Coulomb energy is \( E_n^C = -C_F^2 \alpha_s^2/4n^2 \). \( \delta E_n^{(k)} \) stands for corrections of order \( \alpha_s^k \). The first and second order corrections can be found in \( \text{Ref.} 1, 4, 5, 6 \) for arbitrary \( n \).

The \( O(\alpha_s^3) \) corrections to the energy levels arise from several sources: (i) matrix elements of the NextLO operators of the effective Hamiltonian between Coulomb wave functions; (ii) higher iterations of the NLO and NNLO operators of the effective Hamiltonian in time-independent perturbation theory; (iii) matrix elements of the NextLO instantaneous operators generated by the emission and absorption of ultrasoft gluons; and (iv) the retarded ultrasoft contribution.

The contributions to \( E_n^{(3)} \) for vanishing \( \beta \)-function were computed for general \( n \) in \( \text{Ref.} 1 \). The corresponding correction to the ground state energy gets contributions from all four sources and reads

\[
\delta E_1^{(3)} \bigg|_{\beta(\alpha_s)=0} = -E_1^C \frac{\alpha_s^3}{\pi} \left\{ \frac{a_1 a_2 + a_3}{32 \pi^2} \right\} C_F^2
\]

\[
+ \left[ \frac{C_A C_F}{2} + \left( \frac{19}{16} + \frac{S(S+1)}{2} \right) C_F^2 \right] a_1
\]

\[
+ \left[ \frac{1}{36} \ln 2 + \frac{L_{\alpha_s}}{6} \right] C_A^2 C_F + \left[ \frac{5}{72} + \frac{10}{3} \ln 2 \right]
\]

\[
+ \frac{4}{3} \left( \ln 2 + L_{\alpha_s} \right) C_A^2 C_F + \left[ \frac{5}{72} + \frac{10}{3} \ln 2 \right]
\]

\[
+ \frac{37}{6} L_{\alpha_s} + \left( \frac{85}{54} - \frac{7}{6} L_{\alpha_s} \right) S(S+1) \right\} C_A C_F^2
\]

\[
+ \left[ \frac{50}{9} \right] + \frac{8}{3} \ln 2 + 3 L_{\alpha_s} - \frac{S(S+1)}{3} \right\} C_F^2
\]

\[
+ \left[ \frac{32}{15} + 2 \ln 2 + (1 - \ln 2) S(S+1) \right] C_F^2 T_F
\]

\[
+ \frac{49 C_A C_F T_F n_l}{36} + \left[ \frac{11}{18} - \frac{10}{27} S(S+1) \right] C_F^2 T_F n_l
\]

\[
+\frac{2}{3} C_F^3 L_1 \right\},
\]

(2)

where the color group invariants are \( C_F = 4/3 \), \( C_A = 3 \), \( T_F = 1/2 \), \( n_l \) is the number of light-quark flavors, \( S \) is the spin quantum number and \( L_{\alpha_s} = -\ln(C_F \alpha_s) \). The numerical value of the QCD Bethe logarithm \( L_F^C = -81.5379 \) can be found in \( \text{Ref.} 1, 4, 5, 6 \). The MS scheme for the renormalization of \( \alpha_s(\mu) \) is implied. The logarithmic \( \ln(\alpha_s) \) part of Eq. (3) has been derived first in \( \text{Ref.} 1, 2, 3 \). The coefficient \( a_1 \) parameterizes the \( \beta \)-loop correction to the Coulomb potential \( (a_1 = 31 C_A/9 - 20 T_F n_l/9 \ldots \text{Ref.} 1 \) \). At present, only Padé estimates of the three-loop MS coefficient \( a_3 \) are available \( \text{Ref.} 1 \). For the bottom and top quark case they read

\[
\frac{a_3}{3} = \begin{cases} 98 & \text{if } n_l = 4, \\ 60 & \text{if } n_l = 5. \end{cases}
\]

(3)

The third order corrections to the ground state energy proportional to the \( \beta \)-function only get contributions from (i) and (ii) and read

\[
\delta E_1^{(3)} \bigg|_{\beta(\alpha_s)} = E_1^C \left( \frac{\alpha_s}{\pi} \right)^3 \left\{ 32 \beta_0^3 L_1^3 + \left[ 40 \beta_0^3 + 12 a_1 \beta_0^2 + 28 \beta_1 \beta_0 \right] L_2^2 + \left[ \left( 16 \pi^2 / 3 \right) + 64 \zeta(3) \right] \beta_0^3 \right\}
\]

\[
+ 10 a_1 \beta_0^2 + \left( 40 \beta_1 + \frac{a_2}{2} + a_2 + 8 \pi^2 C_A C_F \right)
\]

\[
+ \left( \frac{21 \pi^2}{2} - \frac{16 \pi^2}{3} S(S+1) \right) C_F^2 \beta_0 + 3 a_1 \beta_1
\]

\[
+ 4 \beta_2 \right\} L_3 + \left( -8 + 4 \pi^2 + \frac{2 \pi^4}{45} + 64 \zeta(3) \right)
\]

\[
- 8 \pi^2 \zeta(3) + 96 \zeta(5) \right\} \beta_0^3 + \left( \frac{2 \pi^2}{3} + 8 \zeta(3) \right) a_1 \beta_0^2
\]

\[
+ \left( \frac{8}{3} + \frac{7 \pi^2}{3} + 16 \zeta(3) \right) \beta_1 - \frac{a_2}{8} + \frac{3}{2} a_2 + \left( 6 \pi^2 \right)
\]

\[
- \frac{2 \pi^4}{3} C_A C_F + \left( 8 \pi^2 - \frac{4 \pi^4}{3} + \left( -4 \pi^2 / 3 + 4 \pi^4 / 9 \right) \right)
\]
times $S(1) S(4) C F^2 1 + 2a_1 b_1 + 4 b_2 \right) \right),

\text{(4)}

where $L_\mu = \ln(\mu/(C F a_s m_{\text{q}}))$, $\zeta(z)$ is Riemann’s
$\zeta$-function and $\beta_i$ is the $(i + 1)$-loop coefficient of the QCD $\beta$ function ($\beta_0 = 11 C A/12 - T F n_l/3, \ldots$). The terms proportional to $\beta_3^3$ in
Eqs. (4) have been computed first in [2].

The total result for the third order correction to the ground state energy is given by the sum of Eqs. (2) and (4). Adopting the choice
$\mu = C F a_s(m_{\text{q}})$ one obtains for the bottom and top system (for $S=1$) in numerical form

$$
\delta E_{1}^{(3)} = a_3 E_{1}^\gamma \left[ \begin{array}{c}
\frac{70.590}{56.732} \mid_{n_l=4} \\
\frac{34.229}{26.654} \mid_{n_l=5}
\end{array} \right] + 15.297
\times \ln(a_3) + 0.001 a_3 + \left( \begin{array}{c}
\frac{26.654}{26.654} \mid_{n_l=5}
\end{array} \right) |_{\beta_3^3},

\text{(5)}

where we have separated the contributions arising from $a_3$ and $\beta_3^3$. The only unknown ingredient in our result for $\delta E_{1}^{(3)}$ is the three-loop $\overline{\text{MS}}$ coefficient $a_3$ of the corrections to the static potential entering Eq. (2). Up to now there are only estimates based on Padé approximation which we will use in our analysis. However, our final result only changes marginally even for a rather large deviations of $a_3$ from its Padé estimate.

4. PHENOMENOLOGY OF $t \bar{t}$ THRESHOLD PRODUCTION

Let us focus on the top quark threshold production. (the bottom quark case is considered in [24]). The corresponding experimental data are not yet available and our goal is to present a formula which can be directly used for the top quark mass determination from the characteristics of the cross section of $t \bar{t}$ production near threshold [5]. One has to distinguish the production in $e^+ e^-$ annihilation where the final state quark-antiquark pair is produced with $S = 1$ and in (unpolarized) $\gamma \gamma$ collisions where the dominant contribution is given by the $S$-wave zero spin final state. The nonperturbative effects in the case of the top quark are negligible, however, the effect of the top quark width has to be taken into account properly [2] as the relatively large width smears out the Coulomb-like resonances below the threshold. The NNLO analysis of the cross section [23] shows that only the ground state pole results in the well-pronounced resonance. The higher poles and continuum, however, affect the position of the resonance peak and move it to higher energy. As a consequence, the resonance energy can be written in the form

$$
E_{\text{res}} = 2 m_t + E_{1}^{\text{LO}} + \delta E_{\text{res}}.

\text{(6)}

To compute the shift of the peak position due to the nonzero top quark width $\delta E_{\text{res}}$ we use the result of [24] for the $e^+ e^- \rightarrow t \bar{t}$ and $\gamma \gamma \rightarrow t \bar{t}$ cross sections at NNLO. Numerically for both processes

$$
\delta E_{\text{res}} = 100 \pm 10 \text{ MeV}.

\text{(7)}

This value is rather stable with respect to the variation of all input parameters of our analysis. To evaluate the perturbative contribution we use the result of the previous section up to $N^3$LO. In Fig. 3 the perturbative ground state energy in the next-to-leading (NLO), NNLO and $N^3$LO is plotted as a function of the renormalization scale of the strong coupling constant for $S = 1$. One can see, that the $N^3$LO result shows a much weaker dependence on $\mu$ than the NNLO one. Moreover at the scale $\mu \approx 15 \text{ GeV}$ which is close to the physically motivated scale $\mu_{s}$, the $N^3$LO correction vanishes and furthermore becomes independent of $\mu$, i.e. the $N^3$LO curve shows a local minimum. This suggests the convergence of the series for the ground state energy in the pole mass scheme. Collecting all the contributions we obtain a universal relation between the resonance energy in $t \bar{t}$ threshold production in $e^+ e^-$ annihilation or $\gamma \gamma$ collisions (the result shows very weak spin dependence) and the top quark pole mass

$$
E_{\text{res}} = \left( 1.9833 + 0.007 \frac{m_t - 174.3 \text{ GeV}}{174.3 \text{ GeV}} \right) \times m_t,

\text{(8)}

where the weak nonlinear dependence of Eq. (3) on $m_t$ is taken into account in the second term on the right-hand side of Eq. (3). The central value is computed for $m_t = 174.3 \text{ GeV}$. The analysis of the theoretical uncertainty in Eq. (3) can be found in [2]. Due to the very nice behavior of the perturbative expansion for the ground state
energy we do not expect large higher order corrections to our result. As a consequence the top quark pole mass can be extracted from the future experimental data on $t\bar{t}$ threshold production with the theoretical uncertainty of $\pm 80$ MeV. Thus we find the $N^3$LO corrections to stabilize the behavior of the perturbative series for the ground state energy and to be mandatory for a high precision theoretical analysis.

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