Renormalization-group improvement of the spectrum of hydrogenlike atoms with massless fermions

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We obtain the next-to-next-to-leading-logarithmic renormalization-group improvement of the spectrum of hydrogenlike atoms with massless fermions by using potential NRQED. These results can also be applied to the computation of the muonic hydrogen spectrum where we are able to reproduce some known double logarithms at $O(ma^4)$. We compare with other formalisms dealing with logarithmic resummation available in the literature.


In Ref. [1] (see also Ref. [2]), the renormalization-group (RG) improvement of the heavy quarkonium spectrum for the equal mass case was obtained within the potential NRQCD (PNRQCD) formalism [3]. This result was compared with that of Ref. [4] (see also Refs. [5,6]) obtained within the VNRQCD formalism [7] and disagreement was found. This disagreement is potentially important as it propagates to different observables, for example, $t\bar{t}$ production near threshold, where it is claimed [8] that the resummation of logarithms plays an important role. For instance, the matching coefficient of the electromagnetic current, which is a necessary ingredient in these calculations, is different [9,6]. Nevertheless, for the known logarithms at next-to-next-to-leading [10] and next-to-next-to-next-to-leading order [11], both calculations happen to agree with each other.

In order to try to clarify this issue, we consider the simplified problem of a hydrogen-like system coupled to $n_f$ light (massless) fermions in QED. We then obtain the next-to-next-to-leading-logarithm (NNLL) RG scaling of the spectrum of this system. In principle, these results can be applied to muonic hydrogen. In this case, the electron is replaced by the muon, $n_f=1$ and the remaining light fermion is the electron (which we take to be massless for simplicity or, at most, of $O(ma^2)$, where $m$ is the mass of the muon). In this situation, we are able to compare, in certain limits, with finite $O(ma^6\ln^2)$ results already available in the literature [12]. Our results agree with these calculations.

The computation closely follows the procedure of Ref. [1] to which we refer for details. Here we just write the main formulas necessary to set up the notation and the results.

The first step is to obtain the RG improved matching coefficients of the NRQED [13] Lagrangian at one loop and up to $O(1/m^2)$ [$m$ is the mass of the massive lepton (the muon for the muonic hydrogen) and the mass of the nucleus is sent to infinity in this paper].

The NRQED Lagrangian including light fermions reads at $O(1/m^2)$ (up to field redefinitions) [13–15]

$$\mathcal{L} = \mathcal{L}_\gamma + \mathcal{L}_f + \mathcal{L}_\mu + \mathcal{L}_p + \mathcal{L}_{\mu p},$$

where $\mu$ is the Pauli spinor that annihilates the fermion, $N_p$ is the Pauli spinor that annihilates the nucleus, $iD_0 = i\partial_0 - gA_0$, $i\mathbf{D} = i\nabla + g\mathbf{A}$, $\mu^\dagger = \bar{l}_i\gamma^\mu l_i$, and $\mathcal{L} = N_p iD_0^\dagger N_p$.

$$\mathcal{L}_\gamma = -\frac{i}{2} F^{\mu\nu} F_{\mu\nu},$$

$$\mathcal{L}_f = \sum_{i} \bar{l}_i i\mathbf{D}l_i + c^{(3)} g^2 \frac{8}{8m^2} \sum_{i} \bar{l}_i \gamma^\mu l_i \bar{l}_j \gamma_\mu l_j + c^{(4)} g^2 \frac{8}{8m^2} \sum_{i} \bar{l}_i \gamma^\mu \gamma_5 l_i \bar{l}_j \gamma_\mu \gamma_5 l_j,$$

$$\mathcal{L}_\mu = \mu^\dagger \left[ iD_0 + c_k \frac{D^2}{2m} + c_s \frac{\mathbf{B} \cdot \mathbf{B}}{2m} + c_{FG} \frac{\mathbf{D} \cdot (\mathbf{E} - \mathbf{E} \cdot \mathbf{D})}{8m^2} + i\sigma_{5g} \frac{\mathbf{D} \times (\mathbf{E} - \mathbf{E} \times \mathbf{D})}{8m^2} \right] \mu + c^{(4)} g^2 \frac{8}{8m^2} \sum_{i} \mu^\dagger \mu \bar{l}_i \gamma_0 l_i,$$

$$\mathcal{L}_p = N_p iD_0^\dagger N_p,$$
where \( iD_p^0 = i\partial_0 + gZ\alpha_0 \) and
\[
\mathcal{L}_{\mu\mu} = \frac{d_\mu}{m^2} \mu^\mu \mu N_\rho^\mu N_\rho + \frac{d_v}{m^2} \sigma \mu N_\rho^\mu \sigma N_\rho. \tag{6}
\]

We have also included the \( D_j^j/m^3 \) term above since it will be necessary in the evaluation of the spectrum once the power counting is established. Moreover, we will consider that the kinetic term matching coefficients are protected by reparametrization invariance (\( \gamma = \gamma = 1 \)) [16], however, we will often keep them explicit for tracking purposes.

By definition, NRQED has an ultraviolet cutoff \( \nu_{NR} = \{\nu_p, \nu_s\} \) satisfying \( m\nu \ll \nu_{NR} \ll m \). \( \nu_p \) is the ultraviolet (UV) cutoff of the relative three-momentum of the heavy fermion and antifermion. \( \nu_s \) is the UV cutoff of the three-momentum of the photons and light fermions. The derivation of the scale dependence of the matching coefficients with respect the UV cutoffs of the theory is identical to that in Ref. [1]; in particular, the fact that no dependence of \( \nu_p \) appears at this order. In principle, the running of \( c^\mu \) and \( c^\mu \) could be deduced from the results of Refs. [15,14] by taking care of the changes of the color structure. Since we are only interested in the computation of the spectrum at NNLL accuracy, their contribution will vanish at this order as far as the spectrum is concerned (\( c^\mu \) appears in the equation of \( c_D \) but the running of \( c^\mu \) is zero at LL accuracy). Therefore, the relevant RG equations in our case read
\[
\frac{d}{d\nu_s} c_D = -\frac{\alpha}{\pi} \left[ \frac{8}{3} c_8 + \frac{1}{2} \frac{c_{\nu}}{c_3} \right],
\]
and zero otherwise.

By taking the matching conditions at the scale \( m \): \( c_8 = c_F = c_s = c_D = 1 \) and \( \{d\} = 0 \), we can obtain the solution of the RG equations. We only explicitly display those that will be necessary later on [we define \( z = [\alpha(\nu_s)/\alpha(m)]^{b_0} \approx 1 - \frac{1}{2} \alpha(\nu_s) \ln(\nu_s/m), \quad b_0 = -\frac{3}{2} \ln T_F/n_F \) with \( T_F = 1 \)]
\[
c_F(\nu_s) = 1,
\]
\[
c_s(\nu_s) = 1,
\]
\[
c_D(\nu_s) = 1 - \frac{16}{\pi} \ln z,
\]
\[
d_F(\nu_s) = 0,
\]
\[
d_s(\nu_s) = 0.
\tag{8}
\]

The above results are a necessary step towards the RG improvement of PNRQED with the matter content described above, which we consider in what follows. PNRQCD is defined by the cutoff \( \nu_{PRQCD} = \{\nu_p, \nu_{us}\} \), where \( \nu_p \) is the cutoff of the relative three-momentum of the heavy fermions and is such that \( m\nu \ll \nu_p \ll m \), and \( \nu_{us} \) is the cutoff of the three-momentum of the photons and light fermions with \( m\nu^2 \ll \nu_{us} \ll m\nu \).

The PNRQED Lagrangian reads as follows \( (iD_5^0 = i\partial_0 + g(Z-1)A_0) \):
\[
L_{PNRQED} = \int d^3x d^3x_s \left\{ iD_5^0 - c_5 \frac{p^2}{2m} + c_4 \frac{p^4}{8m^3} \right. \\
- V(0) - \frac{V(1)}{m} - \frac{V(2)}{m^2} + g V_A(x \cdot E(x,t)) \right\} S(x,x_s) + \sum_{\mu = 0}^3 \int d^3x d^3x_s \left[ F_{\mu \nu} F_{\mu \nu} \right]. \tag{9}
\]

where \( x \) and \( X \), and \( p \) and \( P \) are the relative and center-of-mass coordinate and momentum, respectively. All the gauge fields in Eq. \( 9 \) are functions of the center-of-mass coordinate and the time \( t \) only. We have explicitly written only the terms relevant to the analysis at the NNLL.

We now display the structure of the matching potentials \( V(0), V(1), \) and \( V(2) \), which are the relevant ones to our analysis. At order \( 1/m^0 \), we have the static potential
\[
V(0) \equiv -Z \frac{\alpha}{r}. \tag{10}
\]
In principle, at order \( 1/m \), we may have a potential scaling as \( V(1)/m \sim 1/(m^2) \). Nevertheless, it vanishes at the order we are working with. It would give, at most, \( O(ma^0) \) corrections to the spectrum in a finite order calculation and the running equations would not mix it. Therefore, for the purposes of this paper, we approximate
\[
V(1) = V(1)/m^0 = 0. \tag{11}
\]

At order \( 1/m^2 \), to the accuracy we aim at, \( V(2) \) has the structure
\[
\frac{V(2)}{m^2} = \frac{\pi Z D_5^2}{m^2} \delta^{(3)}(r) + \frac{3ZD_5^2}{2m^2} \frac{1}{r^2} L_1 \cdot S_1, \tag{12}
\]
where \( S_1 = \sigma_1/2 \). In principle, one may consider more structures for the \( 1/m^2 \) potential but, since they will not contribute at the accuracy we aim at and in order to focus the problem as much as possible, we will set them to zero in what follows, as we have done for the \( 1/m \) potential.

The coefficients \( \bar{V} = \{\alpha_{\nu_s, D_5, \ldots} \} \) contain some \( \ln r \) dependence once higher order corrections to their leading (non-vanishing) values are taken into account. In particular, we will have expressions such as \( \delta^{(3)}(r) \ln^n r \). This is not a well-defined distribution and should be understood as the Fourier transform of \( \ln^n r \). Nevertheless, in order to use the same notation for all the matching coefficients, and since it will be sufficient for the purposes of this paper, namely, to resum the leading logarithms, we will use the expression \( \delta^{(3)}(r) \ln^n r \), although it should always be understood in the sense given above.

By studying the UV behavior of PNRQED it is possible to obtain the scale dependence of the coefficients of the potentials \( V \). The discussion closely follows that of Ref. [1] to
which we refer for details. Here we just mention the main points. The potentials have the following structure:

\[
\begin{align*}
\tilde{V}(d(v_p, v_s, m), c(v_s, m), v_s, v_{US}, r) &= \tilde{V}(v_p, m, v_{US}, r) \\
&= \tilde{V}(v_p, v_{us}).
\end{align*}
\]

(13)

In particular,

\[
\nu_s \frac{d}{d
u_s} \tilde{V} = 0.
\]

(14)

Moreover, at the accuracy we aim, at we also get

\[
\nu_p \frac{d}{d
u_p} \tilde{V} = 0.
\]

(15)

Therefore, we obtain

\[
\tilde{V}(v_p, v_{us}) = \tilde{V}(v_{us})
\]

(16)

and we only have to compute the \(v_{us}\)-scale dependence.

The \(v_{us}\)-scale dependence could be obtained along the same lines as in Ref. [1]. We obtain in this specific case,

\[
\nu_{us} \frac{d}{d
u_{us}} \alpha_s \approx -\beta_0 \frac{\alpha_s^2}{2\pi},
\]

(17)

\[
\nu_{us} \frac{d}{d
u_{us}} D^{(2)}_{dS}(v_{us}) = -\frac{4}{3} \frac{\alpha_{v}(v_{us})}{\pi} V_{A}^2 \alpha (r^{-1}),
\]

and zero for the other potentials.

Equations (14), (15), and (17) provide the complete set of RG equations at the desired order. By using Eqs. (14) and (15), we obtain

\[
\tilde{V} = \tilde{V}(d(1/r, m), c(1/r, m), v_s = 1/r, v_{us}, r).
\]

(18)

We now need the initial condition in order to solve the us RG equations, i.e., the matching conditions. We fix the initial point at \(v_{us} = 1/r\). In summary, we need to know the static potential with \(O(\alpha^3)\) accuracy, the \(1/m\) potential with \(O(\alpha^2)\) accuracy, the \(1/m^2\) potentials with \(O(\alpha)\) accuracy, and \(V_A\) with \(O(1)\) accuracy at \(v_{US} = 1/r\). For the nonvanishing potentials, they read

\[
\alpha_v(r^{-1}) = \alpha_v(r^{-1}) \left[ 1 + (a_1 + 2 \gamma_E \beta_0) \frac{\alpha_v(r^{-1})}{4\pi} + \gamma_E(4a_1 \beta_0 + 2 \beta_4 + \left( \frac{\pi^2}{3} + 4 \gamma_E^2 \right) \beta_0 + a_2 \frac{\alpha_v(r^{-1})}{16 \pi^2} \right],
\]

\[
D^{(2)}_{d}(r^{-1}) = \alpha_v(r^{-1}) \frac{c_D(r^{-1})}{2},
\]

\[
D^{(2)}_{LS}(r^{-1}) = \frac{\alpha_v(r^{-1})}{3} c_S(r^{-1}),
\]

where \(\beta_4 = -4 T_f n_f\) and the values of \(a_1\) and \(a_2\) can be easily obtained from the QCD results [17] by taking \(C_f \rightarrow 1\), \(C_A \rightarrow 0\) and \(T_f \rightarrow 1\).

We now have all the necessary ingredients to solve the RG equations. The RG improved potentials read

\[
\alpha_v(v_{us}) = \alpha_v(r^{-1}),
\]

\[
D^{(2)}_{dS}(v_{us}) = \frac{\alpha_v(r^{-1})}{3} \frac{c_D(r^{-1})}{2},
\]

This completes the RG evaluation of the PNRQED Lagrangian at NNLL.

With the above results we can obtain the energy with NNLL accuracy. The discussion goes similar to that in Ref. [1]. All the large logarithms can be obtained from the potential terms. Once the potentials are introduced in the Schrödinger equation, the \(\ln^n(1/r)\) terms produce \(\ln^n(m\alpha)\) terms plus subleading contributions \([\ln^{n-1}(m\alpha), \ldots]\) within the LL resummation counting. The expectation value of the potential terms is \(v_{us}\)-scale dependent. This scale dependence is canceled by the ultraviolet scale dependence of ultrasoft loops. The typical scale in these integrals is of the order \(m\alpha^2\). Therefore, the logarithms of the ultrasoft loops get minimized by setting \(v_{us} \sim m\alpha^2\) and all the large logarithms get encoded in the potential contributions. Finally, one obtains the following correction to the NNLO energy expression:

\[
\delta E_{n, i,j}^{pot}(v_{us}) = E_n \frac{a_z^2 \delta_{0, j}}{3n} \left[ 1 - \frac{16}{21} \frac{\alpha_v(v_{us})}{\beta_0} \right] - 3(c_B - 1).
\]

(21)

where \(E_n = -m Z^2 \alpha_z^2/(2n^3)\) and the scale \(v_z\) in \(z\) and in the NRQED matching coefficients has been fixed to the soft scale \(v_s = 2a_n^{-1}\), where \(a_n^{-1} = m Z \alpha_z(2a_n^{-1})/n\). \(\alpha_z\) is also understood at the soft scale \(v_s = 2a_n^{-1}\) unless the scale is specified. The \(v_{us}\)-scale dependence of Eq. (21) cancels against contributions from us energies. Since \(m\alpha^2\) is the next relevant scale, their effective role will be to replace \(v_{us}\) by \(m\alpha^2\) (up to finite pieces that we are systematically neglecting) in Eq. (21). In particular, we take \(v_{us} = -E_n\). As expected, Eq. (21) with \(v_{us} = -E_n\) reproduces the well-known hydrogenlike \(O(m\alpha^4 \ln \alpha)\) correction but, indeed, Eq. (21) gives all the \(O(m\alpha^4 (\alpha \ln \alpha)^n)\) terms for \(n \geq 1\) of the spectrum of the hydrogenlike systems with \(n_f\) massless fermions. After adding to Eq. (21) the NNLO result with the normalization point at the same soft scale, \(v_r = 2a_n^{-1}\), that we have used here, the complete NNLO mass is obtained. Note that the above re-
summation of logarithms also correctly accounts for $\ln Z$ terms with the same accuracy.

We have seen that the large logarithms of the spectrum can be obtained from the potential terms by setting $1/r \sim m\alpha$ and $v_{us} \sim m\alpha^2$. The velocity of the nonrelativistic particle is typically $v \sim Z\alpha$. Therefore, it is interesting to consider the scaling of the potentials with respect to $v$ as it will help us to later compare with VNRQED results. In practice, we will consider its scaling with respect to $v = mv$ (therefore $v_{us} = v^2/m$, where

$$\tilde{V}(v_p, m, v_{us}, r)\rightarrow \tilde{V}(m, v_{us}, r)\rightarrow \tilde{V}(m, v^2/m, 1/v) = \tilde{V}(v).$$

(22)

We can now consider its derivative with respect $v$. We will just focus on $D^{(2)}_d$ since it is the only one that has a nontrivial running. We obtain

$$v \frac{d}{dv}D^{(2)}_d = -\frac{\beta_0}{4\pi}c_D(v)\alpha^2(v) + \frac{4}{3} \frac{\alpha^2(v)}{\alpha(n)} \ln \frac{v}{\alpha(m)} - \frac{8}{3} \frac{\alpha(v)}{\pi} \ln \frac{v^2}{m}.$$  

(23)

It is remarkable that the above expression can be rearranged as

$$v \frac{d}{dv}D^{(2)}_d = -\frac{\beta_0}{4\pi}c_D(v)\alpha^2(v) - \frac{8}{3} \frac{\alpha(v)}{\pi} \ln \frac{v^2}{m}.$$  

(24)

There is an evaluation [4] within the VNRQCD framework [7] of the RG improved heavy quarkonium mass when $\Lambda_{QCD} \approx m\alpha^2$. The evaluation performed within the PNRQED framework [1] disagreed with that evaluation. It was noticed there that the disagreement still persisted if one considered a QED-like limit with light fermions by taking $C_f \rightarrow 1$, $C_A \rightarrow 0$, and $T_F \rightarrow 1$. Agreement was found for a QED-like limit without light fermions by taking $C_f \rightarrow 1$, $C_A \rightarrow 0$, $n_f \rightarrow 0$, $T_F \rightarrow 1$. Some errors seem to have been detected in the first versions of these calculations in VNRQCD [18], which may partially explain the difference, in particular, for the $1/m$ potential. In this case, agreement may exist in the limit $C_f \rightarrow 1$, $C_A \rightarrow 0$, and $T_F \rightarrow 1$.

For the evaluation performed in this paper, the computation of the spectrum for the case of hydrogen-like atoms with massless fermions, there exists no analog within the VNRQED framework. Nevertheless, it is possible to guess what would be the result in that formulation by using the rules of Ref. [19], which relate the anomalous dimensions computed here with the ones that should appear in VNRQED. For the specific case of $D^{(2)}_d$, we obtain

$$v \frac{d}{dv}D^{(2)}_d(VNRQED) = \gamma_s + 2 \gamma_u.$$  

(25)

where

$$\gamma_s = -\frac{\beta_0}{4\pi}c_D(v)\alpha^2(v), \quad \gamma_u = -\frac{4}{3} \frac{\alpha(v)}{\pi} \ln \frac{v^2}{m},$$  

(26)

This should be compared with the running in PNRQED obtained above. If we do so, we find that Eqs. (25) and (24) are different. If expanded in $a$, they first differ at $O(\alpha^3\ln^2\alpha)$. This produces a difference in the computation of the mass at $O(m\alpha^4\ln^2\alpha)$. In order to perform an independent check, it would be extremely important that corrections of this order had been computed before. The closest system to the one discussed here corresponds to the muonic hydrogen for which, indeed, corrections to the energy at this order have been computed by Pachucki [12]. In order to compare our results with his evaluation, we have to take the limit $n_f \rightarrow 1$. Moreover, for the real muonic hydrogen, the mass of the light fermion (the electron in this case) is not negligible. However, we can formally consider the situation $m_e \sim m\alpha^2$ (even if for the physical situation $m_e \sim m\alpha$ is closer to reality) in his and our calculation. For the matter of comparison, in our case, this means that, for scales of the order of $m_e$ and $m\alpha^2$, we can use the low-energy electromagnetic coupling $\alpha_{em} \sim 1/137$. This is indeed the parameter expansion used in Pachucki’s calculation. A closer inspection shows that the diagrams that give rise to the large logarithms computed here correspond to the ones drawn in Fig. 4 in Ref. [12]. If we reexpand our result in terms of $\alpha_{em} = \alpha(v_{us})$, we obtain (up to the order of interest and with $v \sim \alpha$)

$$D^{(2)}_d = -\frac{\beta_0}{4\pi}c_D(v)\alpha^2(v) - \frac{8}{3} \frac{\alpha(v)}{\pi} \ln \frac{v^2}{m} + \cdots.$$  

(24)

$$D^{(2)}_d = -\frac{\beta_0}{4\pi}c_D(v)\alpha^2(v) - \frac{8}{3} \frac{\alpha(v)}{\pi} \ln \frac{v^2}{m} + \cdots.$$  

(25)

It is easy to identify the above terms (last equality) within a diagrammatic picture. The first term is the standard Lamb-shift correction one would find for the hydrogen atom and corresponds to the diagrams of Fig. 4 of Ref. [12] without any bubble insertion. The second term corresponds to the first diagram in Fig. 4 of Ref. [12]. The last term corresponds to the second diagram in Fig. 4 of Ref. [12]. Therefore, our result seems to have the correct structure for the $O(m\alpha^3\ln^2\alpha)$ corrections. Let us now go deeper in the comparison with Pachucki’s results. First, we can see that the last term of Eq. (27) can reproduce the analogous Pachucki’s contribution by...
setting $a(\nu_m) = \alpha_{em}$ and $\nu_m = m_e$ (this result depends on the two-loop muon form factor first computed in Ref. [20]). For the second term of Eq. (27), the explicit comparison is a little bit more involved. Nevertheless, it is possible to see that the first term in Eq. (39) of Ref. [12] gives the logarithms of the second term in Eq. (27) since one can make the replacement (as far as the LL contribution is concerned)

$$V_{VP} = -\frac{Z \alpha(\nu_m)}{r} \left[ \frac{\beta_0}{2\pi} a(\nu_m) \ln \frac{mv^2}{m} \right]$$

(28)

for $V_{VP}$, as defined in Ref. [12]. The second term in Eq. (39) of Ref. [12] gives the logarithms due to expanding the wavefunction at the origin $\sim (ma)^3$ [which are naturally written in terms of $\alpha(\nu)$] in terms of $a_{em}$. Therefore, we can trace back all the logarithms of the computation in Ref. [12]. This provides a check of our calculation to a level where it starts to first differ with what would be the VNRQED result. Nevertheless, it may happen that, if the corrections of the VNRQCD results for the equal mass calculation are finally confirmed, they may also explain the different result obtained here.

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1We note that for this diagram both loops factorize. Therefore, no sign of correlation of scales appears at this level of the computation.

In conclusion, we have computed the energy spectrum at NNLL for a hydrogenlike system with $n_f$ massless fermions. We have checked our results at $O(m^2\alpha^3\ln^2)$ by comparing with results already available in the literature [12] for muonic hydrogen and found agreement. We have also compared with what we would expect to be the result in the VNRQED framework based on the rules of Ref. [19] and found disagreement. Finally, we would like to mention that the above results can be useful in checking higher-order logarithms in computations of the spectrum for muonic atoms or alike where the electron can be considered to be a light particle.

**Note added.** Recently a paper appeared [21] where it was pointed out that there was a systematic error in the VNRQCD computations to date and that the diagram Fig. 20b in this reference should be included in such computations. After its inclusion, the corrected $1/m^2$ potential obtained in VNRQCD agrees with the $1/m^2$ potential obtained in PNQCD [1], the replacement $c_D(\nu) \to c_D(\nu^2/m)$ should be done in Eq. (26) and the new result of VNRQED for the muonic hydrogen spectrum agrees with our result.

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