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Expansion of bound-state energies in powers of m/M

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We describe a new approach to computing energy levels of a non-relativistic bound-state of two constituents with masses M and m, by a systematic expansion in powers of m/M. After discussing the method, we demonstrate its potential with an example of the radiative recoil corrections to the Lamb shift and hyperfine splitting relevant for the hydrogen, muonic hydrogen, and muonium. A discrepancy between two previous calculations of $\mathcal{O}(\alpha(Z\alpha)^5 m^2/M)$ radiative recoil corrections to the Lamb shift is resolved and several new terms of $\mathcal{O}(\alpha(Z\alpha)^5 m^4/M^3)$ and higher are obtained.

The theory of non-relativistic bound states in QED remains an important source of information about fundamental physical parameters, like the fine structure constant and the masses of the electron, muon and proton, among many others [1]. Simple atoms, which are being studied in laboratories, differ significantly in the ratios of their constituent masses. Two situations can be distinguished. The first one is the case when the masses of the two constituents of the bound state are equal, with the positronium as the most important example. The second case is a bound state with two very different masses, e.g. hydrogen, muonium, muonic hydrogen. Both situations represent two special limits of a general mass ratio case. In both limits certain simplifications are possible. In the context of this Letter, the case of equal constituent masses was discussed to some extent in [2,3]. In this Letter we consider the case when the masses of the constituents differ significantly from one another.

Our main goal is a practical algorithm which allows a calculation of the bound-state energy levels in a given order of perturbation theory (in α and $Z\alpha$) as an expansion in powers and logarithms of m/M with an arbitrary precision. The opposite situation, i.e. calculation of the energy levels to all orders in α but in a fixed order in the ratio m/M, has been studied in the literature [4–7].

In many practical situations only the first few terms of the expansion in m/M are required. Nevertheless, we believe that it is useful to construct such an algorithm in its generality. First, higher corrections in the ratio m/M might become relevant. For example, in the muonic hydrogen m/M corresponds to $m_\mu/M_p \simeq 0.113$, not a very small parameter. In exotic hadronic atoms, such as pionic hydrogen, that ratio might be even larger. In hydrogen and muonium, where m/M is smaller, the very high precision of experiments warrants a precise computation of the recoil effects. Second, a complete algorithm means that one can obtain the whole series in m/M at once and additional cross checks become possible.

We first recall that non-relativistic bound-state energies can be computed using an effective field theory [8]. In [2,3] we have shown how dimensional regularization facilitates this approach. One has to distinguish two different contributions. The first one is the contribution of the relativistic region in the loop-momentum integrals; in what follows we will refer to these contributions as "hard" contributions. This is usually obtained as a Taylor expansion of the relevant scattering amplitudes in spatial momentum components of external particles (which can be taken on-shell).

Second, there is the so-called "soft" contribution, given by usual time-independent perturbation theory in quantum mechanics. An important point to note is that the soft contribution can in general be easily evaluated for arbitrary masses of constituents. As one can see from the Schrödinger equation, this is so because the essential dynamics of a non-relativistic bound state is governed by the reduced mass of the system rather than by the masses of individual constituents. In this respect, for the soft contributions the relation between the two masses is not very important and once the equal mass case has been solved, the rest follows easily.

Therefore, in the situation where the two masses are different, the real problem is in computing the hard contribution and this is what we are going to discuss in this Letter. We will show that there is a simple way to expand the hard scattering diagrams in powers of m/M. The essential advantage of this method is that it can be

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automated and many terms of the expansion can be easily computed. The only limitation is the available computer power; as a matter of principle, infinitely many terms in the m/M expansion can be obtained. High-performance symbolic algebra software is of great help in such computations (we use FORM [9]).

The remainder of this Letter is organized as follows. First the method is described in detail. Next, we compute the $\alpha(Z\alpha)^5$ radiative recoil corrections to both the Lamb shift and the hyperfine splitting up to the fourth order in the expansion in m/M. Finally, we present our conclusions.

The method we are going to discuss is based entirely on using dimensional regularization. Note that for consistency one also needs the soft contribution in dimensional regularization; as we mentioned earlier this part of the problem is well understood [2,3].

The hard diagrams should be evaluated exactly at the threshold (zero relative velocity of the constituents). For this reason, the relevant Feynman integrals depend on only two scales, m and M. Since we are interested in their expansion in m/M, it is useful to be able to expand the *integrands*, so that only homogeneous one-scale integrals have to be evaluated. Once this is achieved, the calculations simplify dramatically.

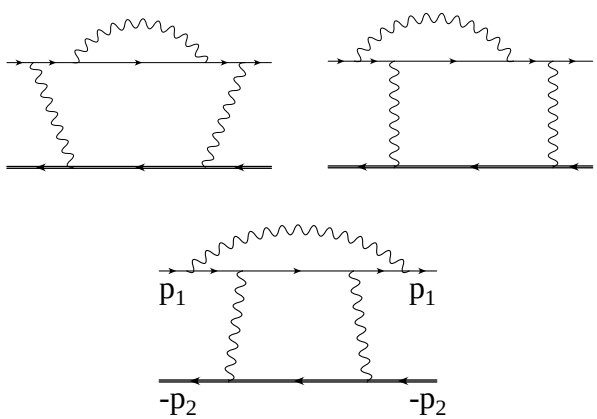

FIG. 1. The forward-scattering radiative-recoil diagrams. The bold line represents the heavy constituent of the bound-state (e.g. proton if we consider hydrogen) and the thin line — the light one (an electron). Diagrams with the crossed photons in the t-channel are not displayed.

Our method is motivated by the known procedure which permits an expansion of Feynman diagrams in large momenta and masses [10–12]. Although originally formulated in a different way, that procedure can be reformulated more practically using the notion of momentum regions. To arrive at the result one should follow a sequence of steps [13]: (1) determine large and small scales in the problem; (2) divide the entire integration volume into regions where each loop momentum is of the order of some of the characteristic scales; (3) in every region perform a Taylor expansion in the parameters which are small in the given region; (4) after the expansion, ignore all the constraints on the regions and perform the integration over the entire integration volume; (5) add the contributions of different regions to obtain the final result. The only step in this sequence which might appear counter-intuitive is the step 4, since one may suspect some double counting. The reason why that does not happen is that the scale-less integrals vanish in the dimensional regularization. This in turn implies that the results obtained from the integrals over different regions are different analytic functions of the parameters of the problem. Below this procedure will be demonstrated in some detail.

To illustrate the method we focus on the last diagram in Fig. 1 and consider the following scalar integral:

$$\int \frac{[\mathrm{d}^D k_1][\mathrm{d}^D k_2]}{(k_1^2)^2 (k_2^2)(k_2^2 + 2p_1 k_2 + i\delta)^2} \times \frac{1}{[(k_1+k_2)^2 + 2p_1(k_1+k_2) + i\delta]\,(k_1^2 - 2p_2 k_1 + i\delta)}. \quad (1)$$

Here $[\mathrm{d}^D k]$ stands for $\mathrm{d}^D k/(2\pi)^D$, $p_1 \equiv mQ$, $p_2 \equiv MQ$, where $Q = (1,0,0,0)$ is the time-like unit vector. Only the relevant infinitesimal imaginary parts of the propagators have been displayed. We are going to illustrate the expansion of the integral in Eq. (1) in powers of m/M following the five steps outlined above.

There are four momentum regions to be considered. In the first one all the momenta are of the order of the large mass M. In this case one can expand the electron propagators in mQk_i. The resulting integrals are all of the form:

$$\int \frac{[\mathrm{d}^D k_1][\mathrm{d}^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1+k_2)^{2a_3}(k_1^2 - 2p_2 k_1)^{a_4}}, \quad (2)$$

with some integer powers a_i. One immediately recognizes that all these integrals are identical with the general two-loop self-energy integrals of the particle with the mass M for which the general solution is known [14].

Next, there are two momentum regions where either $k_1 \sim M$ and $k_2 \sim m$ or $k_1 \sim M$ and $k_2 \sim M$, but $k_1 + k_2 \sim m$. It is then easy to see that after a Taylor expansion in the small variables, the integral factorizes into a product of two simple one-loop integrals.

The fourth region is determined by the condition $k_1 \sim k_2 \sim m$. In this case the heavy particle propagator can be expanded in powers of k_1^2 and in essence it becomes a *static* propagator. The general integral in this case has the form

$$J = \int \frac{[\mathrm{d}^D k_1][\mathrm{d}^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_2^2 + 2p_1 k_2 + i\delta)^{a_3}} \times \frac{1}{[(k_1+k_2)^2 + 2p_1(k_1+k_2) + i\delta]^{a_4}(2p_2 k_1 - i\delta)^{a_5}}. \quad (3)$$

Such integrals represent the only new type required for this calculation and the easiest way to solve them is to

employ the integration-by-parts techniques [15,16]. Any integral J can be algebraically expressed as a combination of the two-loop on-shell self-energy integrals and four new master integrals. The latter are the only integrals we have to compute, but this can be easily accomplished with help of Feynman parameters. The results read

$$J_1^{\pm} = \int \frac{[\mathrm{d}^D k_1][\mathrm{d}^D k_2]}{(k_1 Q - 1 \pm i\delta)(k_2^2 + i\delta)\left[(k_1+k_2)^2 - 1 + i\delta\right]}$$
$$= \frac{1}{(4\pi)^D}\left[2\Gamma(1-\epsilon)\Gamma(3\epsilon-2)B(4\epsilon-3, 2\epsilon-1)\right.$$
$$\left. -(1\mp 1)\sqrt{\pi}\Gamma\left(2\epsilon - \frac{3}{2}\right) B\left(\frac{5}{2} - 3\epsilon, -\frac{1}{2}+\epsilon\right)\right], \quad (4)$$

$$J_2^{\pm} = \int \frac{[\mathrm{d}^D k_1][\mathrm{d}^D k_2]}{(k_1 Q \pm i\delta)(k_2^2 - 1 + i\delta)\left[(k_1+k_2)^2 - 1 + i\delta\right]}$$
$$= \pm\frac{\sqrt{\pi}}{(4\pi)^D}\Gamma\left(2\epsilon - \frac{3}{2}\right) B\left(\frac{5}{2} - 3\epsilon, -\frac{1}{2}+\epsilon\right). \quad (5)$$

Let us add that all momentum regions other than the ones we discussed lead to scale-less integrals and are therefore not relevant. This concludes the construction of our expansion algorithm.

We have applied this algorithm to compute the $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil corrections to the Lamb shift and the hyperfine splitting of a general QED bound state composed of two spin-1/2 particles with the masses m and M. It is well known that in this case the soft contribution is absent and the hard corrections shown in Fig. 1 are the only diagrams we have to consider. We have done the calculation in a general covariant gauge; the cancellation of the gauge parameter dependence serves as a check of the computation.

For the S-wave ground state energy E we define:

$$E = E_{\mathrm{aver}} + \left(\frac{1}{4} - \delta_{J0}\right) E_{\mathrm{hfs}}, \quad (6)$$

where $J = 0, 1$ is the total spin of the two fermions forming the bound state.

For the hyperfine splitting we obtain:

$$\delta E_{\mathrm{hfs}}^{\mathrm{rad\ rec}} \simeq \frac{8(Z\alpha)^4\mu^3}{3mM}\alpha(Z\alpha)\left\{\ln 2 - \frac{13}{4}\right.$$
$$+\frac{m}{M}\left(\frac{15}{4\pi^2}\ln\frac{M}{m} + \frac{1}{2} + \frac{6\zeta_3}{\pi^2} + \frac{17}{8\pi^2} + 3\ln 2\right)$$
$$-\left(\frac{m}{M}\right)^2\left(\frac{3}{2} + 6\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^3\left(\frac{61}{12\pi^2}\ln^2\frac{M}{m} + \frac{1037}{72\pi^2}\ln\frac{M}{m}\right.$$
$$\left. + \frac{133}{72} + \frac{9\zeta_3}{2\pi^2} + \frac{5521}{288\pi^2} + 3\ln 2\right)$$
$$-\left(\frac{m}{M}\right)^4\left(\frac{163}{48} + 6\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^5\left(\frac{331}{40\pi^2}\ln^2\frac{M}{m} + \frac{5761}{300\pi^2}\ln\frac{M}{m} + \frac{691}{240}\right.$$
$$\left.\left. + \frac{9\zeta_3}{2\pi^2} + \frac{206653}{8000\pi^2} + 3\ln 2\right)\right\}, \quad (7)$$

where $\mu = mM/(m+M)$ is the reduced mass of the bound state.

For the spin-independent energy shift we find

$$\delta E_{\mathrm{aver}}^{\mathrm{rad\ rec}} \simeq \alpha(Z\alpha)^5\frac{\mu^3}{m^2}\left\{\frac{139}{32} - 2\ln 2\right.$$
$$+\frac{m}{M}\left(\frac{3}{4} + \frac{6\zeta_3}{\pi^2} - \frac{14}{\pi^2} - 2\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^2\left(-\frac{127}{32} + 8\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^3\left(-\frac{8}{3\pi^2}\ln^2\frac{M}{m} - \frac{55}{18\pi^2}\ln\frac{M}{m} + \frac{47}{36}\right.$$
$$\left. - \frac{3\zeta_3}{\pi^2} - \frac{85}{9\pi^2} - 2\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^4\left(-\frac{55}{24} + 4\ln 2\right)$$
$$+\left(\frac{m}{M}\right)^5\left(\frac{37}{60\pi^2}\ln^2\frac{M}{m} + \frac{29}{900\pi^2}\ln\frac{M}{m} + \frac{1027}{360}\right.$$
$$\left. - \frac{3\zeta_3}{\pi^2} - \frac{370667}{36000\pi^2} - 2\ln 2\right)$$
$$\left. +\left(\frac{m}{M}\right)^6\left(-\frac{67}{20} + 4\ln 2\right)\right\}. \quad (8)$$

To our knowledge the terms $\mathcal{O}(m^3/M^3)$ and higher are new for both E_{hfs} and E_{aver}, while the other terms have been obtained previously. In addition, the coefficient of the $\mathcal{O}(m/M)$ term in Eq. (8) has been subject of some controversy, since two different numerical results have been reported, [17–19] and [20].

Our result for this term,

$$\alpha(Z\alpha)^5\frac{\mu^3}{m^2}\frac{m}{M}\left(\frac{3}{4} + \frac{6\zeta_3}{\pi^2} - \frac{14}{\pi^2} - 2\ln 2\right)$$
$$\simeq -1.32402796\ \alpha(Z\alpha)^5\frac{\mu^3}{m^2}\frac{m}{M}, \quad (9)$$

is in excellent agreement with the numerical result of Ref. [20] where the coefficient $-1.324029(2)$ was obtained.

The discrepancy in the $\mathcal{O}(m^2/M\alpha(Z\alpha)^5)$ corrections to the Lamb shift reported in [17–19] and [20] has been the major source of the theoretical uncertainty in the so-called isotope shift (apart from the uncertainty associated with the proton and deuteron charge radii, see below), i.e. the difference between energies of $2S$ to $1S$ transitions in deuterium and hydrogen:

$$\Delta E = [E(2S) - E(1S)]_D - [E(2S) - E(1S)]_H. \quad (10)$$

Experimentally, ΔE is known with the uncertainty of about 0.15 kHz [21]; the theoretical uncertainty associated with higher order QED effects and with the uncertainties in the electron-to-proton and the electron-to-deuteron mass ratios is about 1 kHz each. On the other hand, the difference in the results of Refs. [17–19] and [20] leads to 2.7 kHz difference in ΔE. Our result for this term, Eq. (9), removes this discrepancy in favor of the result of Ref. [20].

It is well known that the high accuracy of the experimental value of ΔE cannot be used directly because of significant uncertainties in the value of the proton and deuteron charge radii which enter the theoretical formula for ΔE. In this situation the problem is usually turned around and one determines the difference of the charge radii of the proton and deutron using ΔE. Here, we do not pursue this topic any further. The related phenomenology can be extracted from Ref. [21] (see also the recent review [22], where results of Ref. [20] should be used).

We have constructed an efficient algorithm which permits an expansion of the energy levels of a bound state of two constituents with masses m and M in powers of m/M. This expansion is similar to, although not identical with, the asymptotic expansions of Feynman diagrams familiar from particle physics. We have demonstrated the usefulness of this procedure by computing several terms in the m/M expansion for the $\alpha(Z\alpha)^5$ radiative recoil corrections to both the Lamb shift and the hyperfine splitting of a general QED bound state.

Although we have only described a calculation of the radiative recoil corrections, the method is clearly applicable to all other types of corrections relevant for the bound states. In particular, the pure recoil corrections can be treated in a similar way. It remains to work out the details in that case, but the principles are clear.

One of the terms in our result for the radiative recoil corrections to the Lamb shift is the $\mathcal{O}(\alpha(Z\alpha)^5\mu^3/(mM))$ term for which two different numerical results have been previously reported. Our calculation confirms the result of Ref. [20].

Another aspect of this work might be related to higher number of loops. It is clear that the described method can be systematically applied in higher orders. Probably more important, it may facilitate the extraction of terms enhanced by $\ln M/m$ which can be determined from the singularities of the contributions of different expansion regimes. Since those singularities must cancel in the complete result, their coefficients can be found by a partial calculation of the divergent parts of those contributions which can be evaluated most easily.

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