Expansion of bound-state energies in powers of m/M and $(1-m/M)$

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Elaborating on a previous Letter [A. Czarnecki and K. Melnikov, Phys. Rev. Lett. **87**, 013001 (2001)], we use a new approach to compute energy levels of a nonrelativistic bound state of two constituents, with masses m and M, by systematic expansions—one in powers of m/M and another in powers of $(1-m/M)$. Technical aspects of the calculations are described in detail. Theoretical predictions are given for $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil and $\mathcal{O}((Z\alpha)^6)$ pure recoil corrections to the average energy shift and hyperfine splitting relevant for hydrogen, muonic hydrogen, and muonium.

I. INTRODUCTION

Precision studies, both theoretical and experimental, of nonrelativistic QED bound states have historically provided a wealth of information about fundamental physical parameters such as the fine structure constant and the masses of the electron, muon and proton [2]. In order to keep pace with the ever-improving precision of current experiments, increasingly intricate theoretical calculations must be performed. Fortunately, the emergence of new calculational techniques has brought many such calculations within reach.

In a previous Letter [1], we introduced 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, the 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 [3–6]. We illustrated the method by calculating the $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil corrections to the average energy shift and hyperfine splitting of a nonrelativistic QED bound state. This analytic result enabled us to resolve a discrepancy between two previous calculations of $\mathcal{O}(\alpha(Z\alpha)^5 m^2/M)$ corrections to the average energy shift, thereby removing a major source of theoretical uncertainty in the isotope shift (i.e. the difference between the $2S$ to $1S$ transition energies in deuterium and hydrogen).

In this paper we extend our previous results in several ways. For instance, we illustrate how the energy shifts can also be expanded as a series in $(1-m/M)$. Beyond its applicability to situations where $m \sim M$, this expansion method provides a useful cross-check on the comparably more difficult method of expanding in m/M. We also examine the convergence properties of these expansions in order to ascertain some general guidelines about the accuracy of the truncated series that necessarily arise when using these expan-

sions. In addition, we present a calculation of the pure recoil corrections using an expansion in m/M.

The rest of this paper is organized as follows. In Sec. II we discuss the framework of the calculation and our expansion method in general terms. Section III contains a detailed technical description of the calculation. In Sec. IV we present and discuss the results of our calculations for the $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil and $\mathcal{O}((Z\alpha)^6)$ pure recoil corrections to the average energy shift and hyperfine splitting of a generic QED bound state. Our results are summarized in Sec. V. Finally, the Appendix illustrates the techniques with which a class of loop integrals—the so-called eikonal integrals—can be evaluated.

II. FRAMEWORK OF THE CALCULATION

Nonrelativistic bound states can be conveniently described by an effective field theory which exploits a separation in the energy scales m, mv, and mv^2 [7]. This approach is facilitated further by the use of dimensional regularization [8–11]. The basic idea is that the Coulomb potential supplies the dominant interaction and all other interactions provide corrections which can be evaluated using the familiar time-independent perturbation theory of quantum mechanics. These corrections can be divided into two classes.

The first class is that of the so-called "soft" contributions, governed by long-range potential terms. These contributions can be evaluated for arbitrary masses of the constituent particles because the essential soft dynamics of a nonrelativistic bound state, as described by the Schrödinger equation, are characterized by the reduced mass of the system rather than the individual masses of the consituents. As a result, once the soft contributions are obtained in the equal mass case [9,10], the more general mass case follows easily.

The "hard" contributions make up the second class, and these contributions lead to the interactions that can be characterized by $\delta(r)$ potential terms. Such terms result from the relativistic region of loop-momentum integrals, and they are usually obtained as Taylor expansions of scattering amplitudes in terms of the spatial momentum components of the

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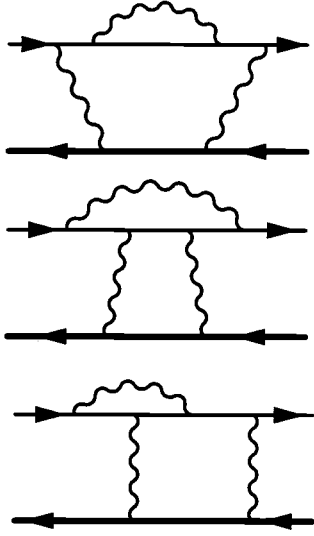
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FIG. 1. The forward-scattering radiative-recoil diagrams. The bold line represents the heavy constituent of the bound state (e.g. a proton if we consider hydrogen) and the thin line represents the light one (an electron). Diagrams with the crossed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

FIG. 2. The forward-scattering pure recoil diagrams.

external particles, which are taken to be on-shell. At lowest order in α, the hard diagrams should be evaluated exactly at threshold, whereby the constituents have zero relative velocity. This implies that the relevant loop-momentum integrals depend on only two scales, m and M. The hard contributions have a much more complicated dependence on the mass scales than the soft contributions do, and this is why we will expand the hard scattering diagrams in powers of either m/M or $(1-m/M)$. By expanding the *integrands*, we are left with only homogeneous, one-scale integrals to evaluate, and this constitutes a substantial simplification. This method lends itself to automation so that many terms of the expansion can be obtained, with the only limitation being set by the available computing power. High-performance symbolic algebra software is of great help in such computations (we use FORM [12]).

Our m/M expansion method is motivated by a procedure in which Feynman diagrams are expanded in large masses and momenta [13–15]. Although this procedure was originally expressed in a different way, it can be reformulated more practically using the notion of momentum regions. The algorithm, which is applied directly to the loop integrals, consists of five steps [16]. First, identify the large and small external scales in the integrals. Second, divide the integration volume into regions so that the momentum flow through any of the internal lines is of the order of one of the external scales. More specifically, the statement $k \sim M$ asserts that $k^2 > m^2$ in Euclidean space. Third, perform Taylor expansions within every region for any individual denominator
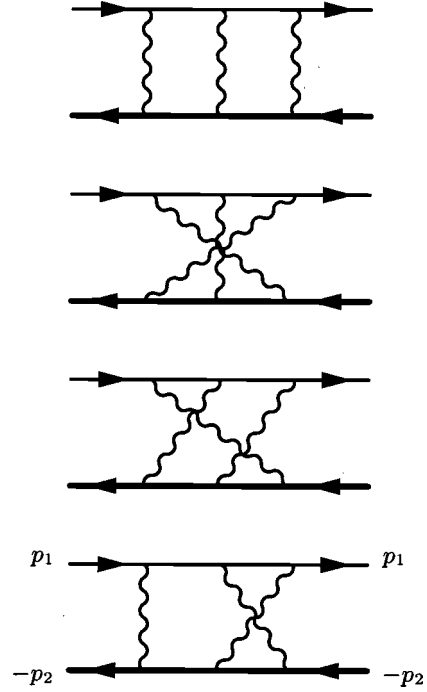
factors (propagators) where the terms within these factors depend differently on the external scales. Fourth, integrate the expanded integrands from every region over the initial integration volume—in other words, ignoring the constraints that identify the regions. Finally, add the contributions arising from the individual regions in order to obtain the final result. The fourth step of this algorithm requires further explanation, since by ignoring the constraints on the individual regions, it may appear as if contributions to the total integral are counted more than once. This does not happen because the extra contributions to the total integral that are introduced by removing the constraints on individual regions can be expressed as scale-less integrals, and scale-less integrals vanish in dimensional regularization. This implies that the integrals from the various regions are different analytic functions of the parameters of the problem. In the next section, we will demonstrate this algorithm in detail.

III. PROCEDURE

In the previous Letter [1], we outlined the expansion procedure for the radiative recoil diagrams. These diagrams are shown in Fig. 1.

We will now describe the expansion procedure using the pure recoil diagrams, since a few additional complications arise. These diagrams are shown in Fig. 2.

To illustrate the method we focus on the last diagram in Fig. 2 and consider the following scalar integral:

$$\int \frac{[d^D k_1][d^D k_2]}{(k_1^2)(k_2^2)(k_1+k_2)^2[(k_1+k_2)^2+2(k_1+k_2)p_1](k_1^2+2k_1p_1)(k_1^2-2k_1p_2+i\delta)(k_2^2+2k_2p_2+i\delta)}. \tag{1}$$

Here $[d^D k]$ stands for $d^D k/(2\pi)^D$, $p_1 \equiv mQ$, and $p_2 \equiv MQ$, 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 five 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

$$\int \frac{[d^D k_1][d^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1+k_2)^{2a_3}(k_1^2-2k_1p_1)^{a_4}(k_2^2+2k_2p_2)^{a_5}}, \tag{2}$$

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 mass M for which the general solution is known [17].

Next, there is a momentum region where $k_1 \sim M$ and $k_2 \sim m$. By using $k_1 \sim M$ to expand the electron propagators we obtain Eq. (2) again. With $k_2 \sim m$, the $(k_1+k_2)^2$ and $(k_2^2+2k_2p_2)$ factors can also be expanded, so that the only denominator factors which depend on k_2 are (k_2^2) and $(2k_2p_2)$. Since we are working at threshold, we have $p_2 \equiv MQ$, which leads to

$$\int \frac{[d^D k_2]}{(k_2^2)^{\alpha}(2k_2p_2+i\delta)^{\beta}} = 0, \tag{3}$$

so that this region provides no contribution to the amplitude for this particular diagram.

The third momentum region has $k_1 \sim M$ and $k_2 \sim M$ but $k_1+k_2 \sim m$. After a Taylor expansion in small variables, the integrals in this region factorize into products of two simple one-loop integrals.

In the fourth region, $k_1 \sim m$ and $k_2 \sim M$. A Taylor expansion in small variables allows the integrals in this region to be factored into one-loop integrals as

$$\int \frac{[d^D k_1]}{(k_1^2)^{a_1}(k_1^2+2k_1p_1)^{a_2}(2k_1p_1)^{a_3}} \int \frac{[d^D k_2]}{(k_2^2)^{a_4}(k_2^2+2k_2p_2)^{a_5}}. \tag{4}$$

The k_2 integral is a trivial one-loop integral. The k_1 integral can be converted to the same simple form, along with integrals like Eq. (3), by multiplying it by factors of

$$1 = \frac{(k_1^2+2k_1p_1)}{(k_1^2)} - \frac{(2k_1p_1)}{(k_1^2)} \tag{5}$$

until either a_2 or a_3 is brought to zero.

The fifth region is characterized by the condition $k_1 \sim k_2 \sim m$. In this case, the heavy particle propagators can be expanded into *static*, or as we will call them, *eikonal*, propagators. The integrals in this region are of the form

$$\int \frac{[d^D k_1][d^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1+k_2)^{2a_3}[(k_1+k_2)^2+2(k_1+k_2)p_1]^{a_4}(k_1^2+2k_1p_1)^{a_5}(2k_1p_2-i\delta)^{a_6}(2k_2p_2+i\delta)^{a_7}}. \tag{6}$$

Notice how the eikonal propagators arising from $(k^2-2kp+i\delta)$ factors acquire $-i\delta$ pole terms. Such terms are important in this region and must be carefully accounted for. The integral in Eq. (6) can be simplified using the identity

$$\frac{1}{(k^2+2kp)(2kp)} = \frac{1}{k^2}\left(\frac{1}{(2kp)} - \frac{1}{(k^2+2kp)}\right). \tag{7}$$

Once one of the seven factors in Eq. (6) has been removed, an identity can be constructed from the observation that the remaining six factors are linearly dependent. Using such an identity, the integrals in this fifth region can be expressed as one of four types of integrals. The first type is the two-loop self-energy integral of a particle with mass m for which the general solution is known [17]. The remaining three types contain eikonal propagators:

$$E_1^{\pm} = \int \frac{[d^D k_1][d^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1-k_2)^{2a_3}(k_2^2+2k_2p_1)^{a_4}(2k_1p_1\pm i\delta)^{a_5}}, \tag{8}$$

$$E_2^{\pm} = \int \frac{[d^D k_1][d^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1^2+2k_1 p_1)^{2a_3}[(k_1+k_2)^2+2(k_1+k_2)p_1]^{a_4}(2k_2 p_1 \pm i\delta)^{a_5}}, \tag{9}$$

$$E_3^{\pm\pm} = \int \frac{[d^D k_1][d^D k_2]}{(k_1^2)^{a_1}(k_2^2)^{a_2}(k_1-k_2)^{2a_3}(2k_1 p_2 \pm i\delta)^{a_4}(2k_2 p_2 \pm i\delta)^{a_5}}. \tag{10}$$

At threshold, the E_3 integrals are exactly zero for similar reasons as are needed to establish Eq. (3). This leaves us with two new types of integrals, E_1 and E_2, required for the recoil calculations. The calculations for radiative recoil diagrams involve E_2 but not E_1 integrals. In Appendix A, we outline the procedure by which the E_1 and E_2 integrals can be evaluated.

We shall now describe a second method of expansion, relevant to the scenario where the two bound-state constituents have similar, but not necessarily equal, masses. Although this scenario is not realized by any common QED bound states, this second expansion can provide a useful check on the first expansion method.

The essential idea is to introduce an expansion parameter

$$y = 1 - \frac{m}{M} \tag{11}$$

so that the external momentum of the light particle, p_1, can be written in terms of y and the external momentum of the heavy particle, p_2, via

$$p_1 = (1-y)p_2. \tag{12}$$

Then, any massive propagator containing p_1 can be expanded, as a series in powers of y, in terms of the corresponding propagators containing p_2:

$$\frac{1}{k^2+2kp_1} = \sum_{n=0}^{\infty} \frac{(2ykp_2)^n}{(k^2+2kp_2)^{n+1}}. \tag{13}$$

As a result, the two-scale general scalar integral in Eq. (1) is expanded, as a series in powers of y, in terms of two-loop

on-shell self-energy integrals. As an additional cross-check, we note that in the limit that the two masses are equal, we have $y=0$, so that the positronium results [9,10] can be recovered from the leading term of this expansion.

Another method has been proposed [18] for dealing with similar problems involving more than one mass-energy-distance scale. Intermediate parameters are introduced to separate various scales and the calculations are performed in four dimensions. An advantage of such an approach is that it avoids various complications arising when working in D dimensions. However, it spoils the homogeneity of integrals and it is not clear whether one can apply integration-by-parts algorithms, which are crucial for larger calculations involving many terms of expansions.

IV. RESULTS AND DISCUSSION

We have applied our algorithms to compute the $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil corrections to the average energy shift and the hyperfine splitting of a general QED bound state composed of two spin-1/2 particles with masses m and M. 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

$$E = E_{\text{aver}} + \left(\frac{1}{4} - \delta_{J0}\right)E_{\text{hfs}}, \tag{14}$$

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

For the hyperfine splitting we obtain

$$\delta E_{\text{hfs}}^{\text{rad rec}} \simeq \frac{8(Z\alpha)^4 \mu^3}{3mM}\alpha(Z\alpha)\left\{ \ln 2 - \frac{13}{4} + \frac{m}{M}\left(\frac{15}{4\pi^2}\ln\frac{M}{m} + \frac{1}{2} + \frac{6\zeta_3}{\pi^2} + \frac{17}{8\pi^2} + 3\ln 2\right) - \left(\frac{m}{M}\right)^2\left(\frac{3}{2} + 6\ln 2\right) \right.$$

$$+ \left(\frac{m}{M}\right)^3\left(\frac{61}{12\pi^2}\ln^2\frac{M}{m} + \frac{1037}{72\pi^2}\ln\frac{M}{m} + \frac{133}{72} + \frac{9\zeta_3}{2\pi^2} + \frac{5521}{288\pi^2} + 3\ln 2\right) - \left(\frac{m}{M}\right)^4\left(\frac{163}{48} + 6\ln 2\right)$$

$$\left. + \left(\frac{m}{M}\right)^5\left(\frac{331}{40\pi^2}\ln^2\frac{M}{m} + \frac{5761}{300\pi^2}\ln\frac{M}{m} + \frac{691}{240} + \frac{9\zeta_3}{2\pi^2} + \frac{206653}{8000\pi^2} + 3\ln 2\right) - \left(\frac{m}{M}\right)^6\left(\frac{577}{120} + 6\ln 2\right) \right\}, \tag{15}$$

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

For the spin-independent energy shift we find

$$
\delta E_{\text{aver}}^{\text{rad rec}} \simeq \alpha(Z\alpha)^5 \frac{\mu^3}{m^2} \left\{ \frac{139}{32} - 2\ln 2 + \frac{m}{M}\left(\frac{3}{4} + \frac{6\zeta_3}{\pi^2} - \frac{14}{\pi^2} - 2\ln 2 \right) + \left(\frac{m}{M}\right)^2 \left(-\frac{127}{32} + 8\ln 2 \right) \right.
$$

$$
+ \left(\frac{m}{M}\right)^3 \left(-\frac{8}{3\pi^2}\ln^2\frac{M}{m} - \frac{55}{18\pi^2}\ln\frac{M}{m} + \frac{47}{36} - \frac{3\zeta_3}{\pi^2} - \frac{85}{9\pi^2} - 2\ln 2 \right) + \left(\frac{m}{M}\right)^4 \left(-\frac{55}{24} + 4\ln 2 \right)
$$

$$
+ \left(\frac{m}{M}\right)^5 \left(\frac{37}{60\pi^2}\ln^2\frac{M}{m} + \frac{29}{900\pi^2}\ln\frac{M}{m} + \frac{1027}{360} - \frac{3\zeta_3}{\pi^2} - \frac{370667}{36000\pi^2} - 2\ln 2 \right) + \left(\frac{m}{M}\right)^6 \left(-\frac{67}{20} + 4\ln 2 \right)
$$

$$
\left. + \left(\frac{m}{M}\right)^7 \left(\frac{199}{70\pi^2}\ln^2\frac{M}{m} - \frac{1759}{7350\pi^2}\ln\frac{M}{m} + \frac{887}{210} - \frac{3\zeta_3}{\pi^2} - \frac{241491119}{18522000\pi^2} - 2\ln 2 \right) \right\}. \tag{16}
$$

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 [19]. The coefficient of the $\mathcal{O}(m/M)$ term in Eq. (16) was the subject of some controversy, since two different numerical results have been reported, Refs. [20–22] and [23].

Our result for this term,

$$
\alpha(Z\alpha)^5 \frac{\mu^3}{m^2} \frac{m}{M} \left(\frac{3}{4} + \frac{6\zeta_3}{\pi^2} - \frac{14}{\pi^2} - 2\ln 2 \right) \simeq -1.32402796\, \alpha(Z\alpha)^5 \frac{\mu^3}{m^2} \frac{m}{M}, \tag{17}
$$

is in excellent agreement with the numerical result of Ref. [23] where the coefficient $-1.324029(2)$ was obtained, and has since been confirmed in an independent analytical calculation [24].

The expansions in m/M of Eqs. (15) and (16) do not yield accurate results for increasing values of m/M, even though an untruncated series can be expected to converge on the interval $m/M \in [0,1)$. The convergence of the terms in the series which we have calculated is depicted in Fig. 3. The upper graph shows the hyperfine splitting calculations as a function of m/M and the lower graph shows the corresponding results for the average energy shift. In both cases, several curves are plotted, each representing the sum of the first N terms of the expansion, where N is shown in the legend. The graphs suggest that more terms in the series would be required to obtain reliable values of the hyperfine splitting for m/M larger than about 0.2; our series for the spin-independent energy shift should be reliable for m/M values up to about 0.5.

The expansion in $y = 1 - m/M$ aims to address the region where m/M is large (i.e., $m \sim M$). For the hyperfine splitting we find

$$
\delta E_{\text{hfs}}^{\text{rad rec}} \simeq \frac{8(Z\alpha)^4 \mu^3}{3mM} \left\{ \left(\frac{3\zeta_3}{4\pi^2} + \frac{7}{8\pi^2} + 2\ln 2 - \frac{79}{32} \right) + \left(1 - \frac{m}{M}\right)\left(-\frac{3\zeta_3}{4\pi^2} - \frac{21}{8\pi^2} - \frac{3}{4}\ln 2 + \frac{25}{96} \right) \right.
$$

$$
+ \left(1 - \frac{m}{M}\right)^2 \left(-\frac{19}{24\pi^2} - \frac{3}{8}\ln 2 - \frac{19}{384} \right) + \left(1 - \frac{m}{M}\right)^3 \left(-\frac{1}{8\pi^2} - \frac{3}{16}\ln 2 - \frac{55}{576} \right)
$$

$$
+ \left(1 - \frac{m}{M}\right)^4 \left(\frac{57}{400\pi^2} - \frac{3}{32}\ln 2 - \frac{2147}{23040} \right) + \left(1 - \frac{m}{M}\right)^5 \left(\frac{11}{40\pi^2} - \frac{3}{64}\ln 2 - \frac{631}{7680} \right)
$$

$$
+ \left(1 - \frac{m}{M}\right)^6 \left(\frac{41389}{117600\pi^2} - \frac{3}{128}\ln 2 - \frac{46679}{645120} \right) + \left(1 - \frac{m}{M}\right)^7 \left(\frac{141709}{352800\pi^2} - \frac{3}{256}\ln 2 - \frac{10561}{161280} \right)
$$

$$
\left. + \left(1 - \frac{m}{M}\right)^8 \left(\frac{5539481}{12700800\pi^2} - \frac{3}{512}\ln 2 - \frac{157753}{2580480} \right) \right\}, \tag{18}
$$

and for the spin-independent energy shift we obtain

$$\delta E_{\text{aver}}^{\text{rad rec}} \simeq \alpha (Z\alpha)^5 \frac{\mu^3}{m^2} \left\{ \left(\frac{9\zeta_3}{2\pi^2} - \frac{35}{4\pi^2} + \frac{31}{12} \right) + \left(1 - \frac{m}{M} \right) \left(-\frac{9\zeta_3}{2\pi^2} + \frac{39}{2\pi^2} - \frac{7}{2}\ln 2 + \frac{45}{32} \right) + \left(1 - \frac{m}{M} \right)^2 \left(\frac{61}{24\pi^2} + \frac{9}{4}\ln 2 - \frac{119}{72} \right) \right.$$

$$+ \left(1 - \frac{m}{M} \right)^3 \left(-\frac{29}{24\pi^2} + \frac{1}{8}\ln 2 + \frac{31}{288} \right) + \left(1 - \frac{m}{M} \right)^4 \left(\frac{233}{600\pi^2} + \frac{1}{16}\ln 2 - \frac{571}{11520} \right)$$

$$+ \left(1 - \frac{m}{M} \right)^5 \left(\frac{509}{1200\pi^2} + \frac{1}{32}\ln 2 - \frac{187}{3840} \right) + \left(1 - \frac{m}{M} \right)^6 \left(\frac{135311}{352800\pi^2} + \frac{1}{64}\ln 2 - \frac{13439}{322560} \right)$$

$$\left. + \left(1 - \frac{m}{M} \right)^7 \left(\frac{39721}{117600\pi^2} + \frac{1}{128}\ln 2 - \frac{1427}{40320} \right) + \left(1 - \frac{m}{M} \right)^8 \left(\frac{5683891}{19051200\pi^2} + \frac{1}{256}\ln 2 - \frac{16901}{552960} \right) \right\}. \tag{19}$$

In Fig. 4 we illustrate the convergence of these series. Both graphs suggest that the terms we have calculated in this expansion should yield reliable results for m/M larger than about 0.15.

Although neither expansion can handle arbitrary values of m and M, the bound-state energy level corrections for any m/M ratio can be reliably calculated with one of the expansions. To illustrate this, we have spliced together the two expansions in Fig. 5. The expansions merge nicely at an m/M value of 0.15, thereby providing a useful check on these methods. It is also important, in the context of future applications of these methods, to have covered the entire range of m/M.

We have also calculated the corresponding $\mathcal{O}((Z\alpha)^6)$ pure recoil corrections. For the hyperfine splitting we obtain

$$\delta E_{\text{hfs}}^{\text{rec hard}} \simeq \frac{8(Z\alpha)^6 \mu^3}{3mM} \left\{ \frac{m}{M} \left(-\frac{1}{2\epsilon} - 6\ln 2 + \frac{5}{12} \right) + \left(\frac{m}{M} \right)^2 \right.$$

$$\times \left(\frac{1}{\epsilon} + \frac{9}{2\pi^2}\ln^2\frac{M}{m} + \frac{27}{2\pi^2}\ln\frac{M}{m} - \ln\frac{M}{m} - \frac{23}{12} \right.$$

$$\left. + \frac{33\zeta_3}{\pi^2} + \frac{93}{4\pi^2} \right) + \left(\frac{m}{M} \right)^3 \left(-\frac{3}{2\epsilon} - 6\ln 2 + \frac{25}{12} \right) \right\}. \tag{20}$$

The divergences in this result are canceled by soft-scale terms, which can be calculated by extending the calculation of [9,10] to the unequal mass case, resulting in

$$\delta E_{\text{hfs}}^{\text{rec soft}} = \frac{(Z\alpha)^6 \mu^5}{m^2 M^2} \left[-\frac{16}{3} \left(\log(2\mu\alpha) - \frac{1}{4\epsilon} \right) \right.$$

$$\left. + 4\frac{mM}{\mu^2} + \frac{230}{27} \right]. \tag{21}$$

Combining the results of Eqs. (20) and (21), we find that the total $(Z\alpha)^6$ pure recoil contribution to the hyperfine splitting is

$$\delta E_{\text{hfs}}^{\text{rec}} \simeq \frac{8(Z\alpha)^6 \mu^3}{3mM} \left\{ \frac{3}{2} + \frac{\mu^2}{mM} \left[\frac{65}{18} - 8\ln 2 + 2\ln(Z\alpha)^{-1} \right. \right.$$

$$+ \left(\frac{m}{M} \right) \left(\frac{9}{2\pi^2}\ln^2\frac{M}{m} + \frac{27}{2\pi^2}\ln\frac{M}{m} - \ln\frac{M}{m} - 12\ln 2 \right.$$

$$\left. - \frac{13}{12} + \frac{33\zeta_3}{\pi^2} + \frac{93}{4\pi^2} \right) + \left(\frac{m}{M} \right)^2 \left(\frac{9}{\pi^2}\ln^2\frac{M}{m} + \frac{27}{\pi^2}\ln\frac{M}{m} \right.$$

$$\left. \left. \left. - 2\ln\frac{M}{m} - 13\ln 2 - \frac{4}{3} + \frac{66\zeta_3}{\pi^2} + \frac{93}{2\pi^2} \right) \right] \right\}. \tag{22}$$

The terms in the first line of Eq. (22) are in agreement with the result first obtained in [25]. The remaining terms, arising solely from the hard-scale contributions in Eq. (20), can be used to obtain an analytic approximation to the function $f(x)$ near $x = 1$ in Eq. (72) of [26].

For the hard contribution to the spin-independent energy shift we find

$$\delta E_{\text{aver}}^{\text{rec hard}} \simeq (Z\alpha)^6 \frac{\mu^3}{m^2} \left\{ \frac{m}{M} \left(4\ln 2 - \frac{7}{2} \right) \right.$$

$$+ \left(\frac{m}{M} \right)^2 \left(\frac{4}{\pi^2}\ln\frac{M}{m} - \frac{8}{3}\ln\frac{M}{m} - \frac{12\zeta_3}{\pi^2} + \frac{3}{\pi^2} + \frac{8}{3} \right)$$

$$+ \left(\frac{m}{M} \right)^3 \left(4\ln 2 - \frac{31}{6} \right) + \left(\frac{m}{M} \right)^4 \left(-\frac{11}{3\pi^2}\ln^2\frac{M}{m} \right.$$

$$\left. \left. - \frac{113}{18\pi^2}\ln\frac{M}{m} - 2\ln\frac{M}{m} - \frac{6\zeta_3}{\pi^2} - \frac{1565}{72\pi^2} + \frac{62}{9} \right) \right\}. \tag{23}$$

The m/M term of this expansion is in agreement with a calculation in Ref. [6]. To our knowledge, the subsequent terms of this expansion are new. In addition, we have calculated these energy level shifts as an expansion in $(1 - m/M)$, but for brevity we shall omit these results.

In spite of the fact that the hard-scale contribution to the average energy shift given by Eq. (23) is finite at this order,
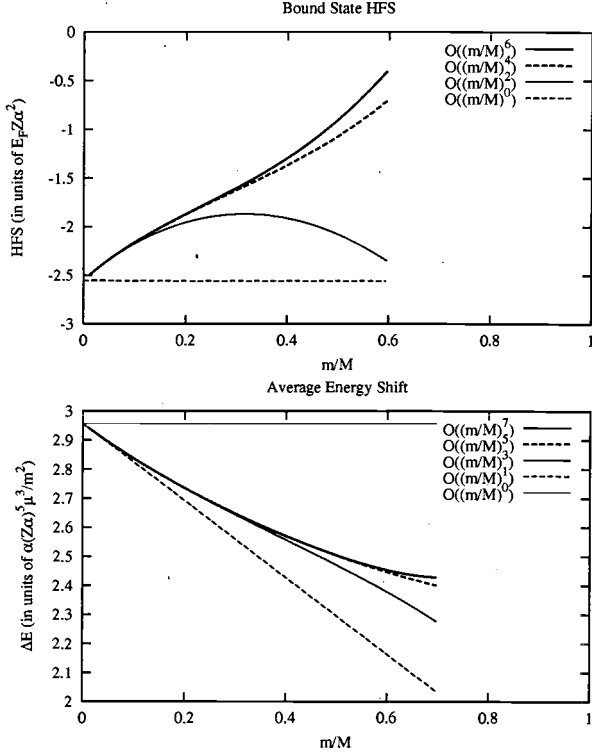
FIG. 3. $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil contributions to the hyperfine splitting and average energy shift in the m/M expansion.

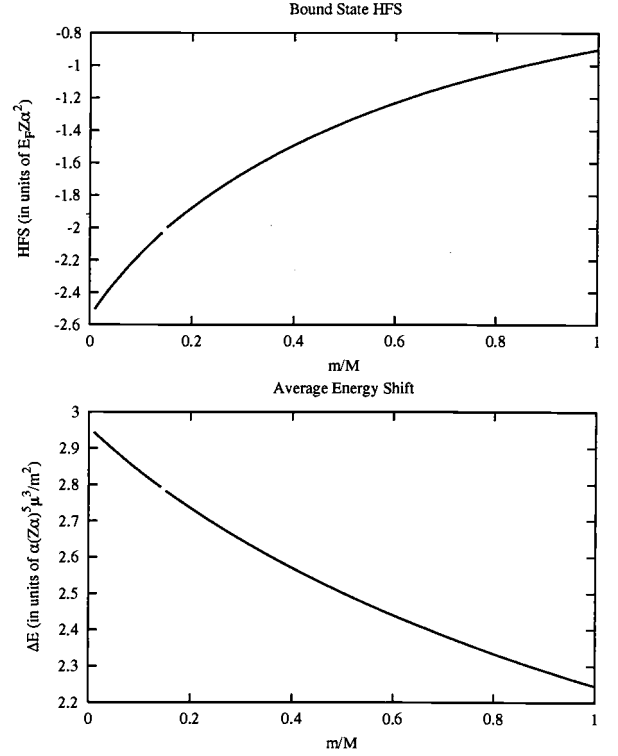

FIG. 5. $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil contributions to the hyperfine splitting and average energy shift for arbitrary values of m and M.

soft contributions are also present and are needed to arrive at the physical result for this quantity. These soft contributions can be obtained by a calculation completely analagous to the one that produced Eq. (21).

V. CONCLUSIONS

We have demonstrated a method by which the corrections to the energy levels of a QED bound state, with constituents of mass m and M, can be expanded in either powers of m/M or $(1-m/M)$. Both expansions are applied directly to the integrands of the loop integrals arising from the hard-scale contributions to the energy shifts. We have demonstrated the utility of these procedures by computing several terms in the expansions for the $\alpha(Z\alpha)^5$ radiative recoil and $(Z\alpha)^6$ pure recoil corrections to both the average energy shift and the hyperfine splitting of a general QED bound state.

Further studies of QED bound-state problems, using the methods described in this paper, might involve higher-order corrections to the energy level shifts. Even in the absence of a complete calculation of such terms, it might be feasible to extract the terms enhanced by one or more factors of $\ln(M/m)$ by examining the singularities of the contributions from different expansion regions. Since these 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.

In a more general context, these expansion techniques are applicable to a plethora of other types of problems involving
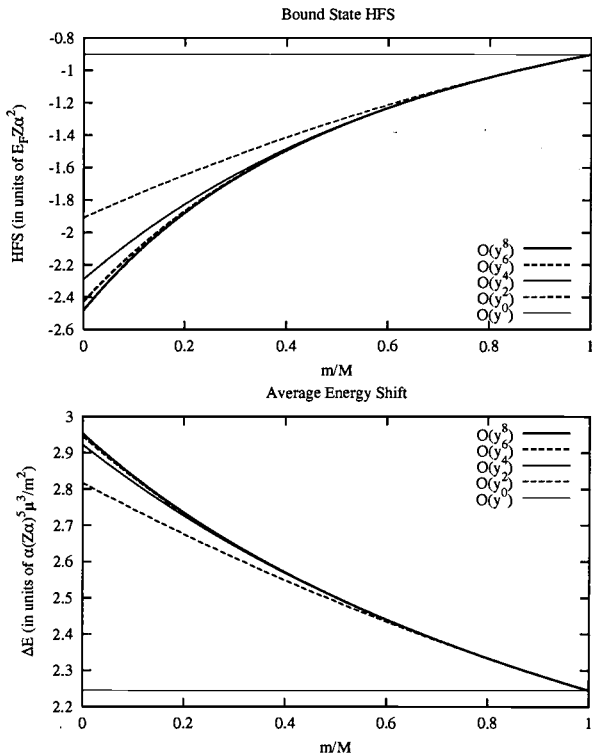

FIG. 4. $\mathcal{O}(\alpha(Z\alpha)^5)$ radiative recoil contributions to the hyperfine splitting and average energy shift in the $1-m/M$ expansion.

multiloop calculations with more than one external scale. Many kinds of superficially disparate physical problems often depend on a few common classes of loop integrals, thereby reducing the number of technical hurdles which restrict the progress of precision calculations in particle physics.

APPENDIX A: CALCULATION OF EIKONAL INTEGRALS

An expansion in powers of m/M typically gives rise to integrals containing eikonal propagators such as $(2kp \pm i\delta)$, arising from expansions in the momentum region where the loop momenta are all $\sim m$. The easiest way to solve them is to employ the integration-by-parts techniques [27,28] so that any integral of the form in Eqs. (8) and (9) 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, and the results read

$$
J_1^\pm = \int \frac{[d^D k_1][d^D k_2]}{(k_1 Q - 1 \pm i\delta)(k_2^2 + i\delta)[(k_1+k_2)^2 - 1 + i\delta]}
$$
$$
= \frac{1}{(4\pi)^D} \left[2\Gamma(1-\epsilon)\Gamma(3\epsilon-2)B(4\epsilon-3, 2\epsilon-1) - (1\mp 1)\sqrt{\pi}\,\Gamma\left(2\epsilon - \frac{3}{2}\right)B\left(\frac{5}{2} - 3\epsilon, -\frac{1}{2} + \epsilon\right) \right],
$$
(A1)

$$
J_2^\pm = \int \frac{[d^D k_1][d^D k_2]}{(k_1 Q \pm i\delta)(k_2^2 - 1 + i\delta)[(k_1+k_2)^2 - 1 + i\delta]}
$$
$$
= \pm \frac{\sqrt{\pi}}{(4\pi)^D}\Gamma\left(2\epsilon - \frac{3}{2}\right)B\left(-\frac{1}{2} + \epsilon, -\frac{1}{2} + \epsilon\right).
$$
(A2)

Please note that there is a typographical error for $J_2^\pm$ in [1]. For clarity, we now outline the process by which these master integrals are calculated.

Starting with J_1^+, we can Wick rotate the momenta and subsequently ignore the poles. After shifting k_1 to $k_1 - k_2$ and using the identity

$$
\frac{1}{A^\alpha B^\beta} = \frac{1}{B(\alpha,\beta)}\int_0^\infty d\lambda \frac{\lambda^{\beta-1}}{[A+B\lambda]^{\alpha+\beta}},
$$
(A3)

we have

$$
J_1^+ = \int \frac{[d^D k_1][d^D k_2]}{k_2^2} \int_0^\infty \frac{d\lambda}{[k_1^2 + 1 + \lambda(k_1 Q - k_2 Q + 1)]^2}.
$$
(A4)

The k_1 integral can be evaluated, after completing the square and using $Q^2 = -1$, so that

$$
J_1^+ = \frac{\Gamma(\epsilon)}{(4\pi)^{D/2}}\int_0^\infty d\lambda \int \frac{[d^D k_2]}{k_2^2\left(\frac{\lambda^2}{4} + \lambda + 1 - \lambda k_2 Q\right)^\epsilon}.
$$
(A5)

Introducing a second parameter from the identity in Eq. (A3), the k_2 integral can be evaluated, yielding

$$
J_1^+ = \frac{\Gamma(2\epsilon-1)}{(4\pi)^D}\int_0^\infty d\lambda \int_0^\infty d\rho\, \rho^{-\epsilon}\left(\frac{\rho\lambda^2}{4} + \frac{\lambda^2}{4} + \lambda + 1\right)^{1-2\epsilon}.
$$
(A6)

With the substitution

$$
\rho = 4z \frac{(\lambda/2 + 1)^2}{\lambda^2},
$$
(A7)

we can readily integrate over the remaining parameters to obtain the result for J_1^+ in Eq. (A1). The evaluation of J_2^+ starts by introducing a Feynman parameter to combine and integrate over the k_2-dependent factors, and is followed by the introduction of a parameter from the identity in Eq. (A3).

Turning to J_1^-, we note that the $-i\delta$ pole term in the eikonal propagator prohibits a Wick rotation. Instead, the identity

$$
\int_{-\infty}^\infty \frac{dx}{x - a \pm i\delta} = P\int_{-\infty}^\infty \frac{dx}{x-a} \mp i\pi\delta(x-a),
$$
(A8)

with respect to the k_1^0 integral, allows us to write

$$J_1^- = J_1^+ + \Delta J_1 \qquad (A9)$$

with

$$\Delta J_1 = 2\pi i \int \frac{[d^D k_1][d^D k_2]\delta(k_1^0 - 1)}{(k_2^2 + i\delta)[(k_1 + k_2)^2 - 1 + i\delta]}. \qquad (A10)$$

A Feynman parameter can be introduced to evaluate the k_2 integral in ΔJ_1. After performing the k_1^0 integral, we have

$$\Delta J_1 = \frac{-2\pi\Gamma(\epsilon)}{(4\pi)^{D/2}(2\pi)^D} \int_0^1 dx$$

$$\times \int \frac{d^{D-1}\mathbf{k}}{[x - x(1-x) + x(1-x)\mathbf{k}^2]^\epsilon}, \qquad (A11)$$

where $\mathbf{k}$ denotes the $(D-1)$-dimensional spatial momentum associated with k_1. Working in hyperspherical coordinates, and using

$$\int d^{D-1}\Omega = \frac{2\pi^{(D-1)/2}}{\Gamma\left(\dfrac{D-1}{2}\right)}, \qquad (A12)$$

we obtain

$$\Delta J_1 = -\frac{4\sqrt{\pi}}{(4\pi)^D} \frac{\Gamma(\epsilon)}{\Gamma\left(\dfrac{3}{2} - \epsilon\right)} \int_0^1 dx \int_0^\infty \frac{k^{D-2}dk}{[x^2 + x(1-x)k^2]^\epsilon}, \qquad (A13)$$

with $k = |\mathbf{k}|$. With the substitution

$$k = \sqrt{\frac{x}{1-x}}z, \qquad (A14)$$

the x and z integrals can be evaluated in terms of B functions, yielding the result in Eq. (A1). The evaluation of J_2^- proceeds in a similar fashion.

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